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A SINGULARLY PERTURBED BOUNDARY VALUE PROBLEM MODELLING A SEMIC--ETC(U)

MAY 82 P A MARKOWICH, C A RINGHOFFER

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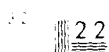
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MRC Technical Summary Report #2388

A SINGULARLY PERTURBED BOUNDARY VALUE
PROBLEM MODELLING A SEMICONDUCTOR DEVICE

Peter A. Markowich, Chr. A. Ringhofer,
Siegfried Selberherr and Erasmus Langer

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MODELLING A SEMICONDUCTOR DEVICE

Peter A. Markowich*, Chr. A. Ringhofer**,
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ABSTRACT

This paper is concerned with the static, one-dimensional modelling of a semiconductor device (namely the pn-junction) when a bias is applied. The governing equations are the well known equations describing carrier transport in a semiconductor which consist of a system of five ordinary differential equations subject to boundary conditions imposed at the contacts. Because of the different orders of magnitude of the solution components at the boundaries, we scale the components individually and obtain a singular perturbation problem.

We analyse the equilibrium case (zero bias applied) and set up approximate models, posed as singularly perturbed second order equations, by neglecting the hole and electron current densities. This makes sense for small forward bias and for reverse bias.

For the full problems we prove an a priori estimate on the number of electron-hole carrier pairs and derive asymptotic expansions (as the perturbation parameter tends to zero) by setting up the reduced system and the boundary layer system. We prove existence theorems for both systems and use the asymptotic expansion to solve the model equations numerically and analyse the dependence of the solutions on the applied bias.

AMS (MOS) Subject Classifications: 34B15, 34E15

Key Words: Nonlinear Differential Equations, Singular Perturbations,
Semiconductors

Work Unit Number 1 (Applied Analysis)

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SIGNIFICANCE AND EXPLANATION

This paper is concerned with the mathematical modelling of a diode. This device consists of a semiconductor, say silicon, which is doped with positive ions on one side and with negative ions on the other side. We take the standard equations describing hole-electron transport in a semiconductor and reformulate them (by scaling of the dependent and the independent variables) as a singularly perturbed system of ordinary differential equations (that means at least one derivative of a dependent variable is multiplied by a small parameter, called perturbation parameter) subject to boundary conditions. The dependent variables are the electrostatic potential, the carrier densities and the current densities.

The advantage of the singular perturbation approach is that asymptotic expansions of solutions (as the perturbation parameter tends to zero) can be derived and used for the analysis and numerical solution of the model equations.

We present an analytical and numerical study of the equations (using the asymptotic expansions) and investigate how the behavior of the model depends on the bias applied to the contacts of the diode.



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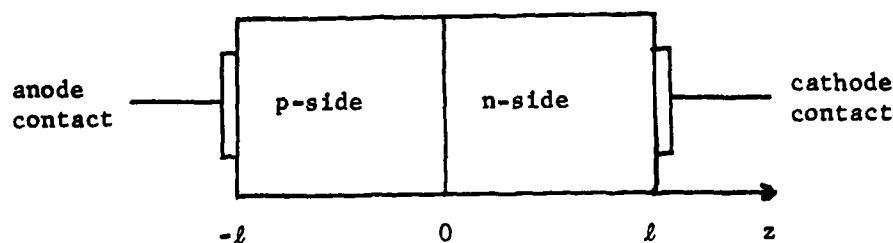
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A SINGULARLY PERTURBED BOUNDARY VALUE PROBLEM
MODELLING A SEMICONDUCTOR DEVICE

Peter A. Markowich*, Chr. A. Ringhofer**,
Siegfried Selberhern*** and Erasmus Langer***

1. Introduction

This paper is concerned with the following physical situation. A semiconductor (for example silicon) is doped with acceptor atoms (positive ions) in the left side (p-side), with donor atoms (negative ions) in the right side (n-side) and a bias $U = U_A - U_C$ is applied to the contacts:



The device is assumed to have characteristic length $2l = 5 \times 10^{-3}$ cm and the pn-junction is assumed to be in the middle. A description of the physics of this device can be found in Ashcroft and Mermin (1976) and R.A. Smith (1978).

The model equations governing the static one-dimensional case are (see de Mari (1968)):

- | | | |
|--|-----------------------------------|-------|
| (a) $\psi'' = \frac{q}{\epsilon}(n-p-C(z))$ | Poisson's equation | |
| (b) $n' = \frac{\mu_n}{D_n} n \psi' + \frac{1}{qD_n} J_n$ | electron current relation | |
| (c) $p' = -\frac{\mu_p}{D_p} p \psi' - \frac{1}{qD_p} J_p$ | hole current relation | (1.1) |
| (d) $J_n' = qR(n,p)$ | continuity equation for electrons | |
| (e) $J_p' = -qR(n,p)$ | continuity equations for holes | |

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for $-l \leq z \leq l$ subject to the boundary conditions

$$\begin{aligned}
 (a) \quad \psi(-l) &= U_T \ln \frac{n_1}{p(-l)} + U_A && \text{(anode)} \\
 (b) \quad \psi(l) &= U_T \ln \frac{n(l)}{n_1} + U_C && \text{(cathode)} \\
 (c) \quad n(\pm l)p(\pm l) &= n_1^2 \\
 (d) \quad n(\pm l) - p(\pm l) - C(\pm l) &= 0,
 \end{aligned} \tag{1.2}$$

where we require that $\psi, n, p, J_n, J_p \in C^1([-l, l])$, $\psi \in C^2([-l, 0) \cup (0, l])$ holds.

The set of full equations (dynamic, two-dimensional) can be found in Van Roosbroeck (1950).

The dependent variables (with units) in (1.1) are

ψ	potential (V)
n	electron density (cm^{-3})
p	hole density (cm^{-3})
J_n	electron current density (A/cm^2)
J_p	hole current density (A/cm^2) .

Of course, we only admit solutions fulfilling $n \geq 0, p \geq 0$.

All parameters in (1.1), (1.2) (except $C(z)$) and the temperature ($T \approx 300\text{K}$) are assumed to be constant. The function $C(z)$, called doping profile (or impurity distribution), is given by

$$C(z) = N_D^+(z) - N_A^-(z) \quad (\text{cm}^{-3}) \tag{1.3}$$

where N_D^+ is the donor density and N_A^- is the acceptor density. $C(z)$ is negative in $[-l, 0)$ (p-side) and positive in $(0, l]$ and is assumed to jump at $z = 0$ (abrupt junction). In this paper we also assume that $C(z)$ is odd, that $|C(z)|$ varies moderately and

$$0 < M \leq C(z) \sim C(l) = 10^{17} \text{ cm}^{-3}, \quad z \in (0, l]. \quad (1.4)$$

The physical meaning (and numerical value) of the other parameters in (1.1), (1.2) is given in Table 1.

TABLE 1: PARAMETERS AT $T \sim 300\text{K}$

Parameter	Physical Meaning	Numerical Value
q	elementary charge	10^{-19} Asec
ϵ	dielectricity constant	$10^{-12} \text{ Asec/Vcm}$
μ_n	electron mobility	$10^3 \text{ cm}^2/\text{Vsec}$
μ_p	hole mobility	$10^3 \text{ cm}^2/\text{Vsec}$
D_n	electron diffusion constant	$25 \text{ cm}^2/\text{sec}$
D_p	hole diffusion constant	$25 \text{ cm}^2/\text{sec}$
n_i	intrinsic number	10^{10} cm^{-3}
$U_T = \frac{D_n}{\mu_n} = \frac{D_p}{\mu_p}$	thermal voltage	0.025 V

Temperature- and space-dependent modelling of these parameters can be found in Langer, Selberherr and Mader (1981) and Selberherr (1981).

$R(n, p)$ in (1.1)(d), (e) is called recombination rate.

We take the Shockley-Read-Hall (SRH) term (see Langer, Selberherr and Mader (1981))

$$R(n, p) = \frac{np - n_i^2}{\tau(n+p) + 2\tau n_i} \quad (\text{cm}^{-3} \text{ sec}^{-1}) \quad (1.5)$$

where $\tau = 10^{-6}$ sec is the electron (and hole) lifetime. Validity restrictions for the SRH-term and various other ways of modelling the recombination rate are given in the above cited references and in R.A. Smith (1978).

The pn-junction is forward biased if $U = U_A - U_C > 0$ and reverse biased if $U < 0$. The boundary conditions (1.2)(c) represent thermal equilibrium at $z = \pm \ell$ and (1.2)(d) represent vanishing space charge (the contacts are assumed to be Ohmic).

The system (1.1), (1.2) was solved numerically by Langer (1980) using a first order difference method and computations for the corresponding two-dimensional model (and for MOS-transistors) and can be found in Selberherr (1981).

The approach taken in this paper is to scale (1.1), (1.2) in such a way that a singular perturbation problem is obtained. This is suited to the problem since the solutions exhibit internal layer structure (at $z = 0$) due to the jump-discontinuity of the doping profile (and since the coefficients in (1.1) are of different orders of magnitude (see Table 1 and (1.4)). Moreover the oddness of $C(z)$ will be used in order to obtain an equivalent problem on the half-interval $[0, \ell]$ (which is of boundary layer type).

The advantage of this procedure is two-fold. Firstly, asymptotic expansions of solutions (as the perturbation parameter converges to zero) can be obtained and secondly the problem can be solved numerically using already developed (high order) methods for boundary layer problems (for example, polynomial collocation as used in this paper). Vasileva and Butuzow (1978), Vasileva and Stelmakh (1977) and D. Smith (1980) proceeded in this way obtaining asymptotic expansions for a simplified problem (they assumed that the recombination rate R is a known function only depending on z).

The paper is organized as follows. In Section 2 we perform the scaling and reformulate (1.1), (1.2) as boundary layer problems on the half-interval. Section 3

is concerned with the case $U = 0$ and with zero-current-density models. In Section 4, we derive asymptotic expansions, demonstrate some qualitative properties of the solution, and explain the numerical results. In Appendix A we give proofs of Theorems on the zero-current-density models and Appendix B is concerned with collocation methods for singular perturbation problems.

2. Reformulation as Singular Perturbation Problem

From (1.2)(c), (d), (1.4) and from $n \geq 0$, $p \geq 0$ we conclude

$$n(\ell) = p(-\ell) = \frac{1}{2}(C(\ell) + \sqrt{C(\ell)^2 + n_1^2}) = C(\ell)(1 + O(10^{-14})) \quad (2.1)(a)$$

$$p(\ell) = n(-\ell) = \frac{1}{2}(-C(\ell) + \sqrt{C(\ell)^2 + n_1^2}) = C(\ell)O(10^{-14}) \quad (2.1)(b)$$

($C(z) = -C(-z)$ holds!) Therefore we set

$$n_s = \frac{n}{C(\ell)}, \quad p_s = \frac{p}{C(\ell)}, \quad D(z) = \frac{C(z)}{C(\ell)} \quad (2.2)(a)$$

and

$$J_{n_s} = \frac{\tau J_n}{4\ell q C(\ell)}, \quad J_{p_s} = \frac{\tau J_p}{4\ell q C(\ell)}, \quad \psi_s = \frac{\psi}{U_T}. \quad (2.2)(b)$$

We also scale the independent variable

$$x = \frac{z}{\ell} \quad (2.3)$$

and get the system

$$\begin{aligned}
\psi'_s &= \frac{\ell^2 C(\ell) q}{U_T \epsilon} (n_s - p_s - D(x)) \\
n'_s &= n_s \psi'_s + \frac{4\ell^2}{rD_n} J_{n_s} \\
p'_s &= -p_s \psi'_s - \frac{4\ell^2}{rD_p} J_{p_s} \quad -1 \leq x \leq 1 \quad (2.4) \\
J'_{n_s} &= \frac{1}{4} \frac{n_s p_s - \left(\frac{n_i}{C(\ell)}\right)^2}{n_s + p_s + 2 \frac{n_i}{C(\ell)}} \\
J'_{p_s} &= -J'_{n_s}
\end{aligned}$$

with boundary conditions

$$\begin{aligned}
(a) \quad \psi_s(-1) &= \ln \left[\frac{\frac{n_i}{C(\ell)}}{p_s(-1)} \right] + \frac{U_A}{U_T} \\
(b) \quad \psi_s(1) &= \ln \left[\frac{\frac{n_s(1)}{n_i}}{\frac{n_i}{C(\ell)}} \right] + \frac{U_C}{U_T} \\
(c) \quad n_s(\pm 1) p_s(\pm 1) &= \left(\frac{n_i}{C(\ell)}\right)^2 \\
(d) \quad n_s(\pm 1) - p_s(\pm 1) - (\pm 1) &= 0.
\end{aligned} \quad (2.5)$$

We set

$$\lambda^2 = \frac{U_T \epsilon}{\ell^2 C(\ell) q}, \quad \gamma^2 = \frac{n_i \ell^2 q}{U_T \epsilon}. \quad (2.6)$$

Using the values for the parameters given in Section 1 and dropping the subscript s , we obtain

$$\begin{aligned}
(a) \quad \lambda^2 \psi'' &= n - p - D(x) \\
(b) \quad n' &= n\psi' + J_n \\
(c) \quad p' &= -p\psi' - J_p \\
(d) \quad J_n' &= \frac{1}{4} \frac{np - \gamma^4 \lambda^4}{n + p + 2\gamma^2 \lambda^2} \\
(e) \quad J_p' &= -\frac{1}{4} \frac{np - \gamma^4 \lambda^4}{n + p + 2\gamma^2 \lambda^2}
\end{aligned} \tag{2.6}$$

for $-1 \leq x \leq 1$ subject to the boundary conditions

$$\begin{aligned}
(a) \quad \psi(-1) &= \psi_-, \quad \psi_- = \ln \frac{\gamma^2 \lambda^2}{p(-1)} + \frac{U_A}{U_T} \\
(b) \quad \psi(1) &= \psi_+, \quad \psi_+ = \ln \frac{n(1)}{\gamma^2 \lambda^2} + \frac{U_C}{U_T} \\
(c) \quad n(\pm 1)p(\pm 1) &= \gamma^4 \lambda^4 \\
(d) \quad n(\pm 1) - p(\pm 1) - (\pm 1) &= 0
\end{aligned} \tag{2.7}$$

where $\lambda^2 = 0.4 \times 10^{-6}$, $\gamma^2 = 0.25$. All quantities in (2.6), (2.7) are dimensionless.

The problem (2.5), (2.6) will be regarded as singular perturbation problem with perturbation parameter λ . Physically, decreasing λ ($\lambda \rightarrow 0+$) means that the concentration of impurities increases ($C(\ell) \rightarrow \infty$). Note that γ^2 is independent of $C(\ell)$.

So far, we have not heavily used the oddness of $C(z)$ (except for (2.1) and (2.7)(d)). For the performed scaling we only have to require that $|C(z)|$ is of the same order of magnitude for all $z \in [-\ell, \ell]$. Now we will use the oddness assumption in order to reduce the problem (2.6), (2.7) to the half-interval $[0, 1]$, thus making the internal layer at $x = 0$ (called depletion-layer or space-charge region in this context) to a boundary layer.

Since only ψ'' , ψ' enter the equations (2.6), the substitution $\psi^*(x) = \psi(x) - \frac{\psi_+ + \psi_-}{2}$ does not change (2.6). Boundary conditions for ψ^* are

$$\psi^*(1) = \psi_+^* = \frac{\psi_+ - \psi_-}{2}, \quad \psi^*(-1) = -\psi_+^* \quad (2.8)$$

and $\psi^*(-1) - \psi^*(1) = \psi_- - \psi_+$ holds. Therefore we can assume (without loss of generality) that

$$\psi_- = -\psi_+ \quad (U_C = -U_A) \quad (2.9)$$

holds. Moreover, given a solution $(\psi, n, p, J_n, J_p)^T$ of (2.6), (2.7) we immediately verify that

$$\begin{aligned} \psi_1(x) &= -\psi(-x) \\ n_1(1) &= p(-x) \\ p_1(x) &= n(-x) \\ J_{n_1}(x) &= J_p(-x) \\ J_{p_1}(x) &= J_n(-x) \end{aligned} \quad (2.9)$$

constitutes another solution, since D is odd and since the SRH recombination rate (1.5) is symmetric in n and p . Therefore we investigate (2.6) on $[0, 1]$ subject to the boundary conditions

$$\begin{aligned} (a) \quad \psi(1) &= \psi_+, \quad \psi(0) = 0 \\ (b) \quad n(1)p(1) &= \gamma^4 \lambda^4, \quad n(1) - p(1) = 1 \\ (c) \quad n(0) &= p(0) \\ (d) \quad J_n(0) &= J_p(0) \end{aligned} \quad (2.10)$$

and continue the solution to $[-1, 1]$ according to (2.9).

We have to expect a boundary layer (as $\lambda \rightarrow 0+$) at $x=0$ in the solution components ψ, ψ', n, p (which are the fast variables), the slow (unperturbed) components J_n, J_p will be uniformly smooth (in λ), no boundary layer will occur at $x=1$ since the reduced solution-manifold ($\lambda=0$), which is given by $\tilde{n} - \tilde{p} - D(x) = 0$, satisfies the (reduced) boundary condition (2.10)(b), given by $\tilde{p}(1) = 0, \tilde{n}(1) = 1$. A proof for this will be given in Section 4.

3. Zero-Current Approximations

We are now concerned with the calculation of the built-in-potential (no voltage is applied, $U_A = U_C = 0$). For simplicity we assume $D \equiv 1$ in this Section.

Setting $J_n \equiv J_p \equiv 0$ we get from (2.6)(b), (c)

$$n = Ae^{\psi}, \quad p = Be^{-\psi}, \quad A, B \in \mathbb{R} \quad (3.1)$$

and from (2.6)(d), (e) we obtain $AB = \gamma^4 \lambda^4$. The boundary conditions (2.10)(a), (b), (c) imply $A = B = \gamma^2 \lambda^2$ and

$$\psi(1) = \ln \left[\frac{1 + \sqrt{1 + 4\gamma^4 \lambda^4}}{2\gamma^2 \lambda^2} \right] =: \psi_+^0(\lambda), \quad \psi(0) = 0. \quad (3.2)$$

Inserting (3.1) into (2.6)(a) gives the equation for the built-in-potential

$$\lambda^2 \psi'' = \gamma^2 \lambda^2 (e^{\psi} - e^{-\psi}) - 1, \quad 0 \leq x \leq 1 \quad (3.3)$$

subject to the boundary conditions (3.2).

This problem is slightly nonstandard since $\psi_+^0(\lambda) \sim \ln \frac{1}{\gamma^2 \lambda^2} \rightarrow \infty$ as $\lambda \rightarrow 0+$ and since the reduced equation (3.3) ($\lambda=0$) is inconsistent.

We obtain the following existence result:

Theorem 3.1. For λ sufficiently small, the problem (3.2), (3.3) has a locally unique solution ψ_0 fulfilling

$$\psi_0(x, \lambda) = \psi_+^0(\lambda) (1 - v_\lambda(\frac{x}{\lambda}) + o(e^{-\frac{C}{\lambda}})) \quad (3.4)$$

where $C > 0$, $v_\lambda(0) = 1$, $v_\lambda(y) \rightarrow 0$ as $y \rightarrow \infty$ and

$$0 < v_\lambda(y) \leq \exp((-1+\delta)y), \quad y \geq \text{const.} \ln \ln \frac{1}{\gamma \lambda^2} \quad (3.5)$$

holds for some $0 < \delta < 1$.

The proof is given in Appendix A.

The corresponding carrier densities n, p are given by (3.1):

$$n_0(x, \lambda) = \exp(-\psi_+^0(\lambda) v_\lambda(\frac{x}{\lambda})) (1 + o(\gamma^2 \lambda^2)) \quad (3.6) (a)$$

$$p_0(x, \lambda) = \gamma^4 \lambda^4 \exp(\psi_+^0(\lambda) v_\lambda(\frac{x}{\lambda})) (1 + o(\gamma^2 \lambda^2)) . \quad (3.6) (b)$$

Since $U = 2U_T(\psi_+^0(\lambda) - \psi_+)$ the pn-junction is forward biased for $\psi_+ < \psi_+^0(\lambda)$ and reverse biased for $\psi_+ > \psi_+^0(\lambda)$.

Theorem 3.1 encourages us to consider approximate problems for (2.6), (2.10) (with $\psi_+ \approx \psi_+^0(\lambda)$) obtained by setting $J_n \equiv J_p \equiv 0$ in (2.6) (b), (c) and ignoring (2.6) (d), (e) (equilibrium models). For the two-dimensional case, this was suggested by Polak et al (1981).

One of the boundary conditions in (2.10) (b), (c) has to be ignored (since (2.10) (b), (c) are consistent with $J_n \equiv J_p \equiv 0$ iff $\psi_+ = \psi_+^0(\lambda)$).

At first we drop the condition $n(1)p(1) = \gamma^4 \lambda^4$ (thermal equilibrium at the contacts) and get from (3.1), (2.10) (b), (c)

$$\lambda^2 \psi'' = \frac{\sinh(\psi)}{\sinh(\psi_+)} - 1, \quad 0 \leq x \leq 1 \quad (3.7)$$

$$\psi(0) = 0, \quad \psi(1) = \psi_+ . \quad (3.8)$$

For $\psi_+ = \psi_+^0(\lambda)$ (3.7), (3.8) gives (3.3), (3.2). Because we require $n \geq 0$, $p \geq 0$, the model (3.7), (3.8) is relevant only for $\psi_+ > 0$.

We get as a generalization of Theorem 3.1:

Theorem 3.2. Assume that λ is sufficiently small and that

$$0 < c_+ \leq \psi_+ < \frac{1-\omega}{2\lambda} \quad (3.9)$$

holds for $\delta < \omega < 1$, $0 < \delta < 1$ independent of λ, ψ_+ . Then the problem (3.7), (3.8) has a locally unique solution $\psi_e = \psi(x, \lambda, \psi_+)$ fulfilling

$$\psi_e = \psi_+ (1 - V_{\psi_+}(\frac{x}{\lambda}) + O(\exp(\frac{(\delta-\omega)}{\lambda}))) , \quad \lambda \rightarrow 0+ \quad (3.10)$$

uniformly in ψ_+ where $V_{\psi_+}(0) = 1$, $V_{\psi_+}(y) \downarrow 0$ as $y \rightarrow \infty$ and

$$0 < V_{\psi_+}(y) \leq \exp((-1+\delta)y) , \quad y \geq \text{const.} \ln \psi_+ \quad (3.11)$$

holds.

The proof is given in Appendix A.

The carrier densities n_e, p_e are calculated from (3.1), (3.7) giving

$$n_e = \frac{e^{\psi_e}}{2 \sinh(\psi_+)} , \quad p_e = \frac{e^{-\psi_e}}{2 \sinh(\psi_+)} . \quad (3.12)$$

For the existence proof (and for $n, p \geq 0$) without uniform asymptotics (in ψ_+) $\psi_+ > 0$ is sufficient.

The width d of the depletion layer of ψ_e is estimated using (3.10):

$$d \leq \text{const.} \lambda \ln \left| \frac{\psi_+}{\lambda} \right| \quad \text{as } \lambda \rightarrow 0+ \quad (3.13)$$

uniformly for ψ_+ satisfying (3.9) where $\text{const.} \approx 1$.

The width of the layer depends logarithmically on ψ_+ for fixed λ .

Figures 1 and 2 show the computed potential $U_T \psi_e$ and the hole density p_e respectively (on the interval $[0, 0.0012]$) for $\psi_+ = 10$, which corresponds to $U \approx 0.306V$ (forward) bias since (for the parameters given in Section 1) $\psi_+^0(\lambda) \approx 16.118$.

The second equilibrium model we investigate is obtained by dropping the symmetry condition $n(0) = p(0)$. From (2.10) (b) we get

$$n(1, \lambda) = \frac{1}{2}(1 + \sqrt{1 + 4\gamma^4 \lambda^4}), \quad p(1, \lambda) = \frac{1}{2}(-1 + \sqrt{1 + 4\gamma^4 \lambda^4}) \quad (3.14)$$

and therefore $A = n(1, \lambda)e^{-\psi_+}$, $B = p(1, \lambda)e^{\psi_+}$. Poisson's equation then reads

$$\lambda^2 \psi'' = n(1, \lambda)e^{(\psi - \psi_+)} - p(1, \lambda)e^{-(\psi - \psi_+)} - 1, \quad 0 \leq x \leq 1 \quad (3.15)$$

subject to the boundary conditions (3.8).

We get

Theorem 3.3. For every $\psi_+ \in \mathbb{R}$ and $\lambda < C(\psi_+)$ the problem (3.15), (3.8) has a locally unique solution ψ_a fulfilling

$$\psi_a = \psi_+ (1 - W_{\psi_+}(\frac{x}{\lambda}) + O(\gamma^4 \lambda^4)) , \quad \lambda \rightarrow 0+ \quad (3.16)$$

where $W_{\psi_+}(0) = 1$, $W_{\psi_+}(y) \rightarrow 0$ as $y \rightarrow \infty$ and

$$0 < W_{\psi_+}(y) \leq \text{const.} \exp((-1 + \delta)y), \quad y \geq 0 \quad (3.17)$$

holds. (For the proof see Appendix A.)

Figures 3 and 4 show the computed curves $U_T \psi_a$ and p_a respectively (on $[0, 0.012]$) for $\psi_+ = 0.4$ ($U = 0.786V$).

FIGURE 1 $U = 0.306V$ ($\psi_+ = 10$)

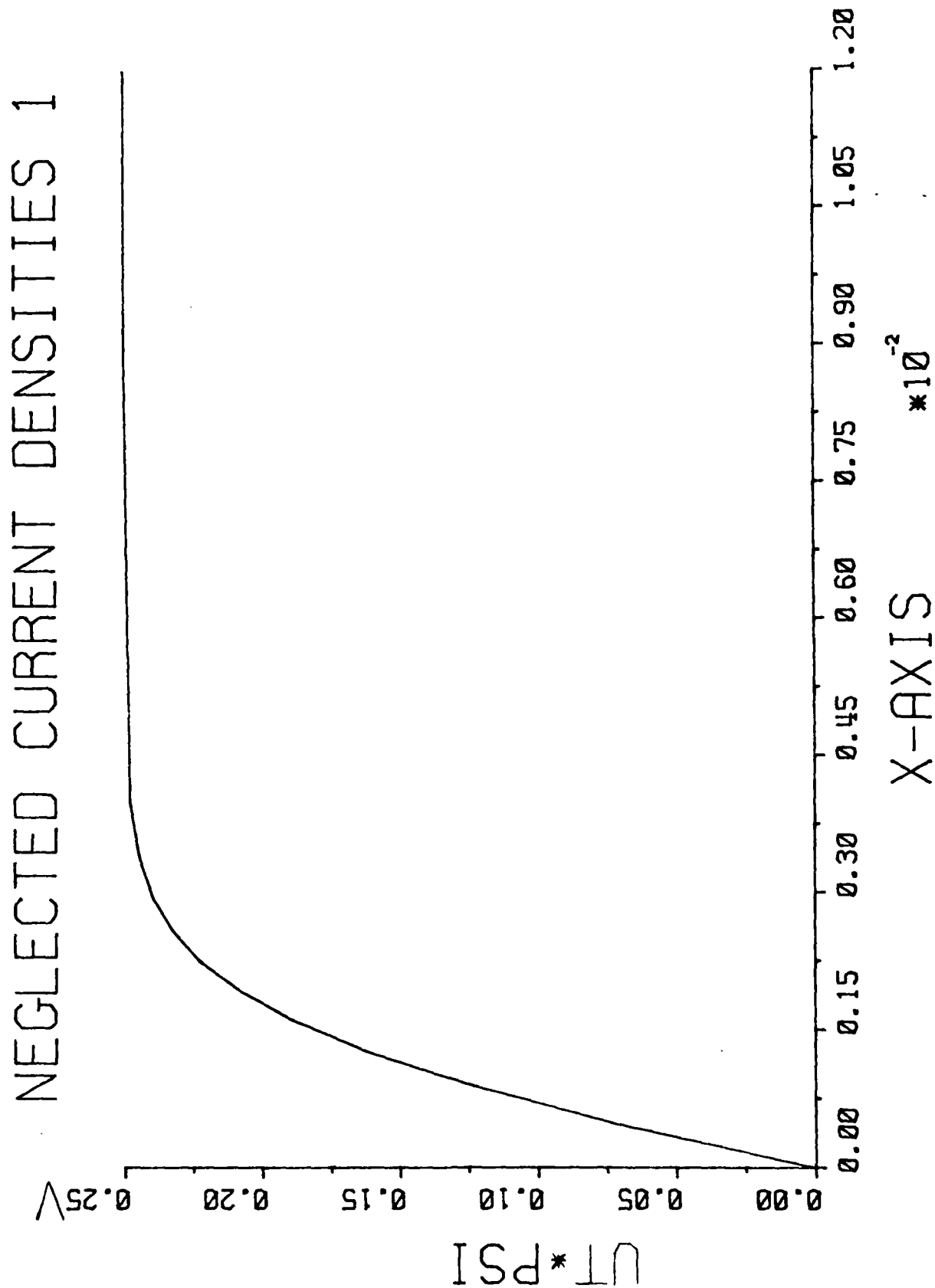


FIGURE 2 $U = 0.306V$ ($\psi_+ = 10$)

NEGLECTED CURRENT DENSITIES 1

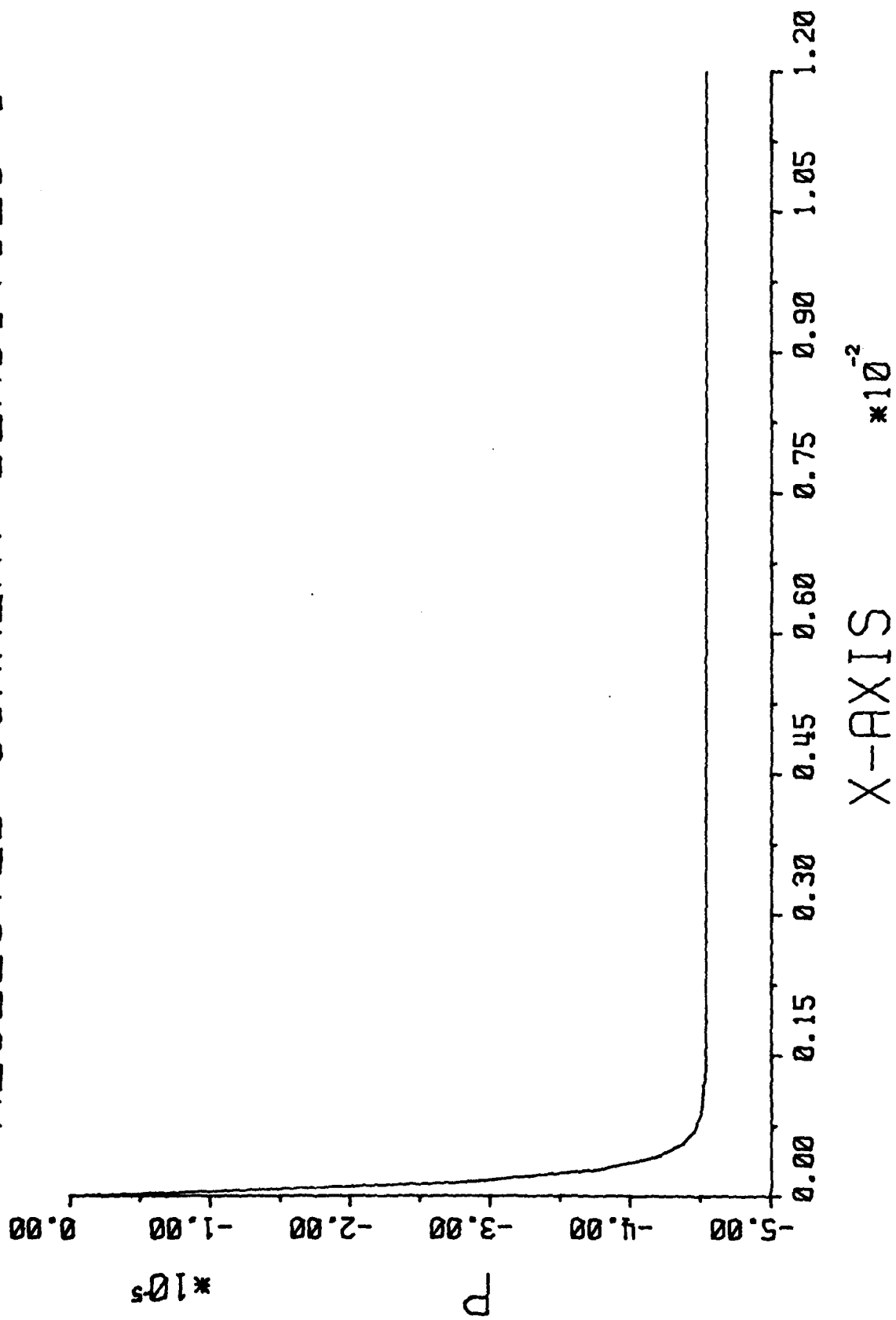


FIGURE 3 $\psi_+ = 0.4$

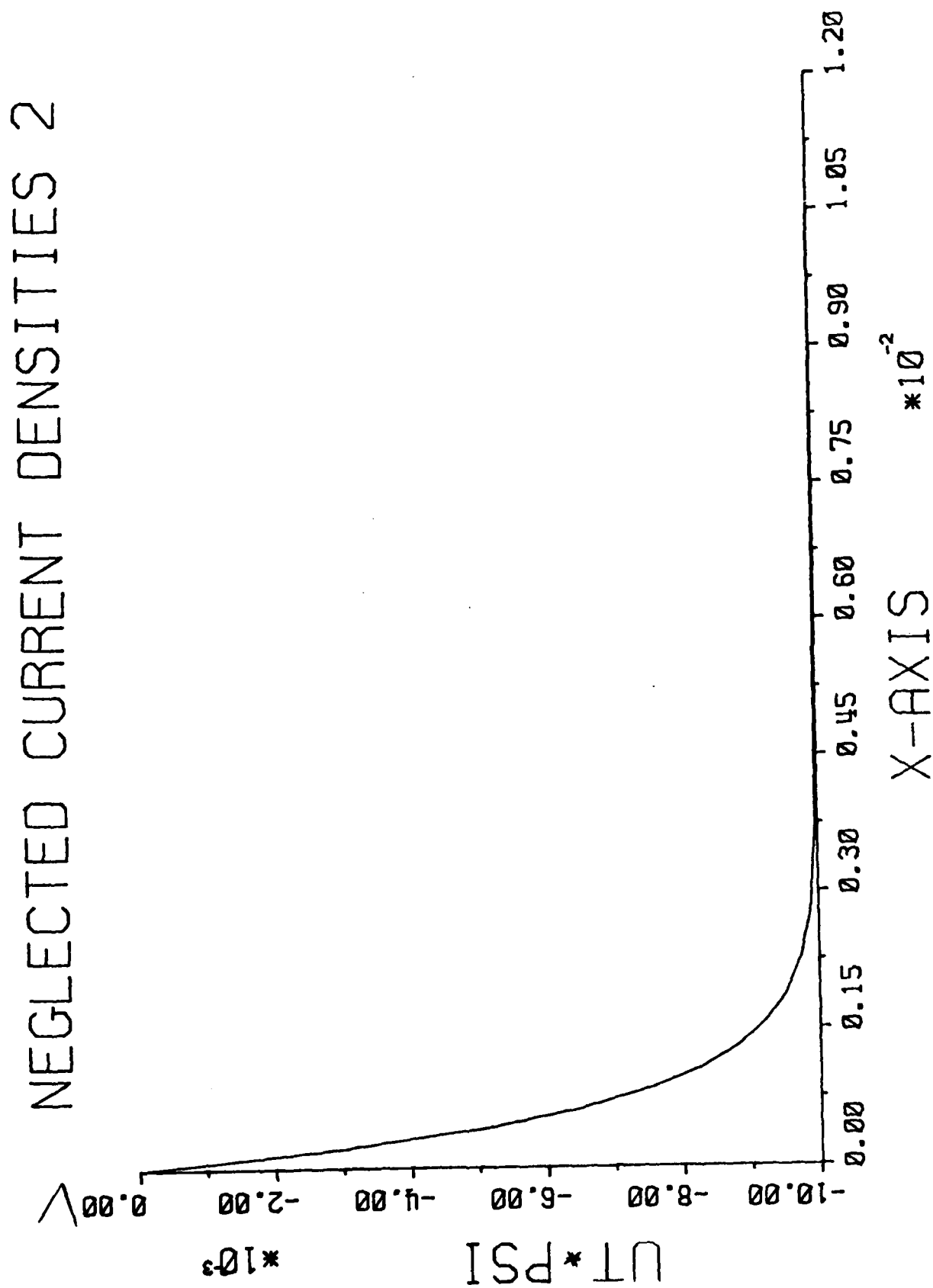
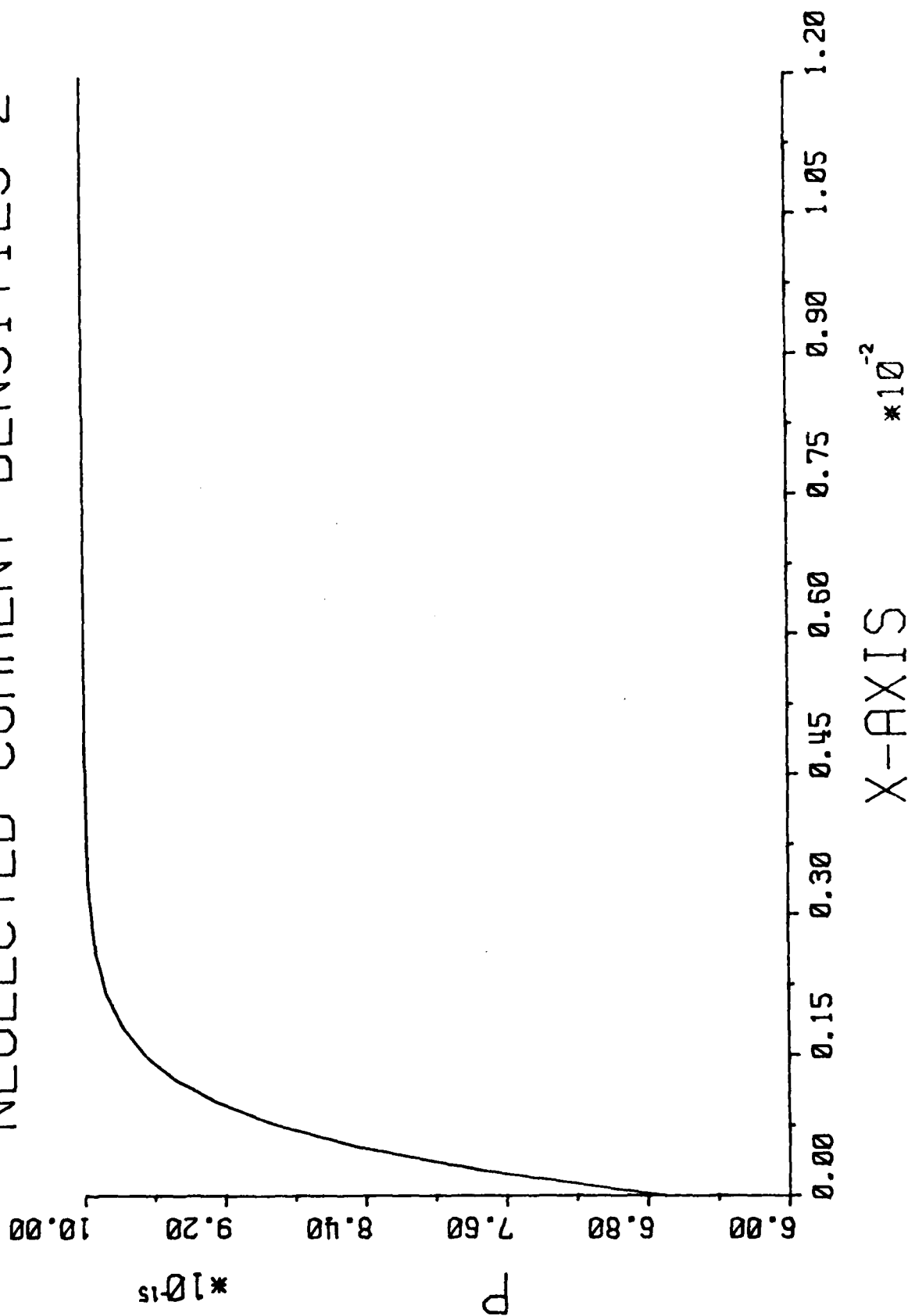


FIGURE 4 $\psi_+ = 0.4$

NEGLECTED CURRENT DENSITIES 2



In order to set up the third possible equilibrium model the vanishing-space-charge condition $n(1) - p(1) = 1$ has to be neglected. Since the analysis for this is quite similar to the analysis of (3.7), (3.8), we do not give details.

A comparison of numerical results obtained for the equilibrium models and the full nonequilibrium model (see next section) shows that the agreement is excellent as long as $U \lesssim 0.3V$ (compare Figures 1 and 15) since then $J \equiv J_n + J_p \lesssim 5 \times 10^{-9}$ holds. The agreement gets rapidly worse as U increases, since J increases exponentially with U (compare Figures 3 and 8).

4. The Nonequilibrium Problem

At first we prove an a priori estimate on the number of electron-hole (carrier) pairs.

Theorem 4.1. Assume that the problem (2.6) and (2.10) has a solution for which $n \geq 0$, $p \geq 0$ holds and J_n, J_p do not change sign in $[0,1]$. Then $J_n \geq 0$, $J_p \geq 0$, $J_n \neq 0$, $J_p \neq 0$ holds for forward bias ($\psi_+ < \psi_+^0(\lambda)$) and $J_n \leq 0$, $J_p \leq 0$, $J_n \neq 0$, $J_p \neq 0$ holds for reverse bias ($\psi_+ > \psi_+^0(\lambda)$). Moreover, the estimate

$$\gamma \lambda^4 \exp\left(-\frac{|U|}{U_T}\right) \leq n(x)p(x) \leq \gamma \lambda^4 \exp\left(\frac{|U|}{U_T}\right), \quad 0 \leq x \leq 1 \quad (4.1)$$

holds.

The assumptions of the Theorem are physically reasonable since n, p are the (scaled) numbers of carriers and since the currents do not change direction in the device.

Proof. It is more convenient to work with the problem (2.6), (2.7) (with $\psi_- = -\psi_+$).

We get from (2.6) (b), (c)

$$n = (E + \int_{-1}^x e^{-\psi(s)} J_n(s) ds) e^{\psi} \quad (4.2) (a)$$

$$p = (F - \int_{-1}^x e^{\psi(s)} J_p(s) ds) e^{-\psi} . \quad (4.2) (b)$$

Obviously $n(-1) = E e^{-\psi_+}$, $p(-1) = F e^{\psi_+}$ holds.

From (2.7) (c) we conclude $EF = \gamma^4 \lambda^4$ and (2.7) (d) gives $E e^{-\psi_+} - F e^{\psi_+} = -1$.

From these equations and from $n \geq 0$, $p \geq 0$ we calculate

$$E = \frac{1}{2} e^{\psi_+} (-1 + \sqrt{1 + 4\gamma^4 \lambda^4}) \quad (4.3) (a)$$

$$F = \frac{1}{2} e^{-\psi_+} (1 + \sqrt{1 + 4\gamma^4 \lambda^4}) . \quad (4.3) (b)$$

We define

$$X = \int_{-1}^1 e^{-\psi(s)} J_n(s) ds \quad (4.4) (a)$$

$$Y = \int_{-1}^1 e^{\psi(s)} J_p(s) ds \quad (4.4) (b)$$

and get from the boundary conditions (2.7) (c), (d) at $x=1$:

$$(E + X)(F - Y) = \gamma^4 \lambda^4 \quad (4.5) (a)$$

$$e^{\psi_+}(E + X) - e^{-\psi_+}(F - Y) = 1 . \quad (4.5) (b)$$

This system of equations has the solutions $X=Y=0$ and

$$X = F - E , \quad Y = X . \quad (4.6)$$

The trivial solution $X=Y=0$ implies $J_n \equiv J_p \equiv 0$ (since J_n, J_p are not allowed to change sign) and this implies $np \equiv \gamma^4 \lambda^4$ and $\psi_+ = \psi_+^0(\lambda)$. Therefore we take (4.6). $X=Y$ is also an immediate consequence of the symmetry (2.9).

A simple calculation shows that $X > 0, Y > 0$ iff $\psi_+ < \psi_+^0(\lambda)$ (forward bias) and $X < 0, Y < 0$ iff $\psi_+ > \psi_+^0(\lambda)$ (reverse bias). This proves the sign-statement on J_n, J_p .

Also

$$n(x)p(x) = (E + \int_{-1}^x e^{-\psi(s)} J_n(s) ds) (F - \int_{-1}^x e^{\psi(s)} J_p(s) ds) \quad (4.7)$$

holds. Therefore we get for forward bias

$$E^2 = E(F-X) \leq n(x)p(x) \leq (E+Y)F = F^2 \quad (4.8)(a)$$

and for reverse bias

$$F^2 = (E+X)F \leq n(x)p(x) \leq E(F-Y) = E^2. \quad (4.8)(b)$$

Using (4.3) and (3.2) gives (4.1).

Expressing (4.1) in the unscaled variables n, p (2.2)(a) gives

$$n_1^2 \exp(-\frac{|U|}{U_T}) \leq n(z)p(z) \leq n_1^2 \exp(\frac{|U|}{U_T}), \quad -\ell \leq z \leq \ell. \quad (4.9)$$

This estimate was anticipated by de Mari (1968). There is numerical evidence that for forward bias $n(z)p(z)$ is close to the upper bound while for reverse bias it is close to the lower bound.

We remark that the explicit form of the recombination rate $R(n, p)$ was not used for the proof of Theorem 4.1 (except for excluding the equilibrium case $J_n \equiv J_p = 0$).

Now we assume that $D \in C^\infty([0, 1])$ and that the solutions of (2.6), (2.7) have an asymptotic expansion given by

$$\begin{pmatrix} \psi(x, \lambda) \\ n(x, \lambda) \\ p(x, \lambda) \\ J_n(x, \lambda) \\ J_p(x, \lambda) \end{pmatrix} \sim \sum_{j=0}^{\infty} \left[\begin{pmatrix} \tilde{\psi}_j(x) \\ \tilde{n}_j(x) \\ \tilde{p}_j(x) \\ \tilde{J}_{n_j}(x) \\ \tilde{J}_{p_j}(x) \end{pmatrix} + \begin{pmatrix} \bar{\psi}_j(\tau) \\ \bar{n}_j(\tau) \\ \bar{p}_j(\tau) \\ \bar{J}_{n_j}(\tau) \\ \bar{J}_{p_j}(\tau) \end{pmatrix} + \begin{pmatrix} \hat{\psi}_j(\sigma) \\ \hat{n}_j(\sigma) \\ \hat{p}_j(\sigma) \\ \hat{J}_{n_j}(\sigma) \\ \hat{J}_{p_j}(\sigma) \end{pmatrix} \right] \lambda^j;$$

$$\tau = \frac{x}{\lambda}, \quad \sigma = \frac{1-x}{\lambda} \quad (4.10)$$

where $\tilde{\psi}_j, \tilde{n}_j, \tilde{p}_j, \tilde{J}_{n_j}, \tilde{J}_{p_j}$ are smooth on $[0, 1]$, $\bar{\psi}_j(\tau), \bar{n}_j(\tau), \bar{p}_j(\tau), \bar{J}_{n_j}(\tau), \bar{J}_{p_j}(\tau)$ and $\hat{\psi}_j(\sigma), \hat{n}_j(\sigma), \hat{p}_j(\sigma), \hat{J}_{n_j}(\sigma), \hat{J}_{p_j}(\sigma)$ are defined on $[0, \infty)$ and decay (exponentially) to zero as $\tau \rightarrow \infty$ and $\sigma \rightarrow \infty$ respectively.

The functions marked with '-' are the boundary layer terms decaying from the left boundary and the functions marked with '^' are the boundary layer terms decaying from the right boundary.

Inserting (4.10) into (2.6), comparing coefficient, setting $\lambda = 0$ and using that the boundary layer terms vanish asymptotically away from the corresponding boundary gives the reduced problem

$$\left. \begin{aligned} (a) \quad 0 &= \tilde{n}_0 - \tilde{p}_0 - D(x) \\ (b) \quad \tilde{n}'_0 &= \tilde{n}_0 \tilde{\psi}'_0 + \tilde{J}_{n_0} \\ (c) \quad \tilde{p}'_0 &= -\tilde{p}_0 \tilde{\psi}'_0 - \tilde{J}_{p_0} \\ (d) \quad \tilde{J}'_{n_0} &= \frac{1}{4} \frac{\tilde{n}_0 \tilde{p}_0}{\tilde{n}_0 + \tilde{p}_0} \\ (e) \quad \tilde{J}'_{p_0} &= -\frac{1}{4} \frac{\tilde{n}_0 \tilde{p}_0}{\tilde{n}_0 + \tilde{p}_0} \end{aligned} \right\} \quad 0 \leq x \leq 1 \quad (4.11)$$

the (zeroth order) left boundary layer system

$$\left. \begin{aligned}
 (a) \quad \dot{\bar{\psi}}_0 &= \bar{n}_0 - \bar{p}_0 \\
 (b) \quad \dot{\bar{n}}_0 &= (\bar{n}_0 + \tilde{n}_0(0)) \dot{\bar{\psi}}_0 \\
 (c) \quad \dot{\bar{p}}_0 &= -(\bar{p}_0 + \tilde{p}_0(0)) \dot{\bar{\psi}}_0 \\
 (d) \quad \dot{\bar{J}}_{n_0} &= 0 \\
 (e) \quad \dot{\bar{J}}_{p_0} &= 0
 \end{aligned} \right\} 0 \leq \tau < \infty \quad (4.12)$$

and the (zeroth order) right boundary layer system

$$\left. \begin{aligned}
 (a) \quad \dot{\hat{\psi}}_0 &= \hat{n}_0 - \hat{p}_0 \\
 (b) \quad \dot{\hat{n}}_0 &= (\hat{n}_0 + \tilde{n}_0(1)) \dot{\hat{\psi}}_0 \\
 (c) \quad \dot{\hat{p}}_0 &= -(\hat{p}_0 + \tilde{p}_0(1)) \dot{\hat{\psi}}_0 \\
 (d) \quad \dot{\hat{J}}_{n_0} &= 0 \\
 (e) \quad \dot{\hat{J}}_{p_0} &= 0
 \end{aligned} \right\} 0 \leq \sigma < \infty \quad (4.13)$$

where ' . ' denotes differentiation with respect to τ or σ respectively.

The boundary conditions (2.10) give

$$\begin{aligned}
 (a) \quad \tilde{\psi}_0(0) + \bar{\psi}_0(0) &= 0 \\
 (b) \quad \tilde{n}_0(0) + \bar{n}_0(0) &= \tilde{p}_0(0) + \bar{p}_0(0) \\
 (c) \quad \tilde{J}_{n_0}(0) + \bar{J}_{n_0}(0) &= \tilde{J}_{p_0}(0) + \bar{J}_{p_0}(0)
 \end{aligned} \quad (4.14)$$

and

$$\begin{aligned}
 (a) \quad \tilde{\psi}_0(1) + \hat{\psi}_0(0) &= \psi_+ \\
 (b) \quad \tilde{n}_0(1) + \hat{n}_0(0) &= 1 \\
 (c) \quad \tilde{p}_0(1) + \hat{p}_0(0) &= 0 .
 \end{aligned} \quad (4.15)$$

since (2.10)(b) reduces to $n(1) = 1$, $p(1) = 0$ for $\lambda = 0$. The systems (4.11), (4.12), (4.13) were obtained by proceeding similarly to O'Malley (1978), Vasileva and Butuzow (1978) and Vasileva and Stelmakh (1977).

From the decay of the layer terms and from (4.12)(d), (e), (4.13)(d), (e), we immediately get

$$\bar{J}_{n_0} \equiv \bar{J}_{p_0} \equiv 0, \quad \hat{J}_{n_0} \equiv \hat{J}_{p_0} \equiv 0 \quad (4.16)$$

J_n, J_p are the slow (unperturbed) components which do not exhibit layer behaviour.

Now we show that no boundary layers at $x = 1$ occur.

Integrating (4.13)(b), (c) gives

$$\hat{n}_0(\sigma) = \tilde{n}_0(1)(e^{\hat{\psi}_0(\sigma)} - 1), \quad \hat{p}_0(\sigma) = \tilde{p}_0(1)(e^{-\hat{\psi}_0(\sigma)} - 1) \quad (4.17)$$

From (4.15)(b) we conclude $\tilde{n}_0(1)e^{\hat{\psi}_0(0)} = 1$ and $\tilde{p}_0(1)e^{-\hat{\psi}_0(0)} = 0$ and therefore $\tilde{p}_0(1) = 0$. This gives

$$\hat{p}_0(\sigma) \equiv 0. \quad (4.18)$$

(4.11)(a) gives $\tilde{n}_0(1) = 1$ and therefore $\hat{\psi}_0(0) = 0$ holds. From (4.13)(a) and from the decay of $\hat{\psi}_0(\sigma)$ we conclude

$$\hat{\psi}_0(\sigma) \equiv 0, \quad \hat{n}_0(\sigma) \equiv 0. \quad (4.19)$$

Boundary layers of order zero can only occur at $x = 0$.

Integrating (4.12)(b), (c) gives

$$\bar{n}_0(\tau) = \tilde{n}_0(0)(e^{\bar{\psi}_0(\tau)} - 1), \quad \bar{p}_0(\tau) = \tilde{p}_0(0)(e^{-\bar{\psi}_0(\tau)} - 1). \quad (4.20)$$

From (4.14)(b) we conclude

$$\tilde{n}_0(0)e^{\tilde{\Psi}_0(0)} = \tilde{p}_0(0)e^{-\tilde{\Psi}_0(0)} \quad (4.21)$$

and since $\tilde{\Psi}_0(0) = -\tilde{\Psi}_0(0)$ ((4.14)(a)) we find the missing boundary condition for the reduced system:

$$\tilde{n}_0(0)e^{-\tilde{\Psi}_0(0)} = \tilde{p}_0(0)e^{\tilde{\Psi}_0(0)} \quad (4.22)$$

The reduced system of equations can now be obtained in closed form from (4.11) by substituting $\tilde{p}_0 = \tilde{n}_0 - D(x)$ into (4.11)(b)-(e) and by eliminating $\tilde{\Psi}'_0$ from (4.11)(b), (c). We drop the subscript 0 and get

$$\left. \begin{aligned} (a) \quad \tilde{n}' &= \frac{\tilde{n}(D'(x) + \tilde{J}_n - \tilde{J}_p) - D(x)\tilde{J}_n}{2\tilde{n} - D(x)} \\ (b) \quad \tilde{\Psi}' &= \frac{D'(x) - (\tilde{J}_n + \tilde{J}_p)}{2\tilde{n} - D(x)} \\ (c) \quad \tilde{J}'_n &= \frac{1}{4} \frac{\tilde{n}(\tilde{n} - D(x))}{2\tilde{n} - D(x)} \\ (d) \quad \tilde{J}'_p &= -\frac{1}{4} \frac{\tilde{n}(\tilde{n} - D(x))}{2\tilde{n} - D(x)} \\ (e) \quad \tilde{p} &= \tilde{n} - D(x) \end{aligned} \right\} 0 \leq x \leq 1 \quad (4.23)$$

subject to the boundary conditions

$$\begin{aligned} (a) \quad \tilde{J}_p(0) &= \tilde{J}_n(0) \\ (b) \quad (\tilde{n}(0) - D(0))e^{2\tilde{\Psi}(0)} &= \tilde{n}(0) \\ (c) \quad \tilde{\Psi}(1) &= \psi_+ \\ (d) \quad \tilde{n}(1) &= 1 \end{aligned} \quad (4.24)$$

From (4.12)(a), (4.20) we get the boundary layer equation

$$\ddot{\bar{\psi}} = \tilde{n}(0)e^{\bar{\psi}} - (\tilde{n}(0) - D(0))e^{-\bar{\psi} - D(0)}, \quad 0 \leq \tau < \infty \quad (4.25)$$

$$\bar{\psi}(0) = -\tilde{\psi}(0), \quad \bar{\psi}(\infty) = 0. \quad (4.26)$$

Higher order terms of the expansion (4.10) can be obtained analogously, however, we will not do so.

At first we prove

Theorem 4.2. Assume that $D(0) > 0$, $\tilde{p}(0) = \tilde{n}(0) - D(0) > 0$. Then the boundary layer equation (4.25), (4.26) has a unique monotonely increasing solution $\bar{\psi}(\tau)$, fulfilling

$$-C_\delta \exp(-\sqrt{(\tilde{n}(0) + \tilde{p}(0))(1-\delta)}\tau) \leq \bar{\psi}(\tau) \leq -C_\delta^{-1} \exp(-\sqrt{(\tilde{n}(0) + \tilde{p}(0))(1+\delta)}\tau) \quad (4.27)$$

on $[0, \infty]$ for any $\delta > 0$ with $C_\delta > 0$.

Proof. The substitution $\bar{\varphi} = -\bar{\psi}$ gives the problem

$$\ddot{\bar{\varphi}} = \tilde{p}(0)e^{\bar{\varphi}} - \tilde{n}(0)e^{-\bar{\varphi} + D(0)} \quad (4.28)(a)$$

$$\bar{\varphi}(0) = \tilde{\psi}(0), \quad \bar{\varphi}(\infty) = 0. \quad (4.28)(b)$$

For $D(0) > 0$, $\tilde{n}(0) - D(0) > 0$ we get $\tilde{\psi}(0) > 0$ from (4.24)(b). Applying Fife's (1973) Lemma 2.1 to (4.28)(a), (b) yields the result.

If $D(0) = 0$ holds, a locally unique solution of (4.25), (4.26) is given by $\bar{\psi} \equiv 0$ which implies $\tilde{n} \equiv \tilde{p} \equiv 0$.

No boundary layers occur if the junction is not abrupt (see also D. Smith (1980) for a simplified model).

The width d of the boundary layer (depletion layer) of ψ can be calculated by taking $C_\delta = \tilde{\psi}(0)$ and by expressing $\tilde{n}(0)$, $\tilde{p}(0)$ in terms of $\tilde{\psi}(0)$.

$$d \sim \lambda \left(D(0) \frac{e^{2\tilde{\psi}(0)+1}}{e^{2\tilde{\psi}(0)-1}} \right)^{-\frac{1}{2}} \left| \ln \left(\frac{\tilde{\psi}(0)}{\lambda} \left(D(0) \frac{e^{2\tilde{\psi}(0)+1}}{e^{2\tilde{\psi}(0)-1}} \right)^{\frac{1}{2}} \right) \right| \quad (4.29)$$

(4.29) should be compared to (3.13) taking into account the Theorem 4.3.

Assuming the validity of the expansion (4.10), $\tilde{p}(0) \geq 0$ (which implies $\tilde{n}(0) \leq D(0) > 0$) is necessary for $p, n > 0$ if λ is sufficiently small since

$$n(0, \lambda) = \tilde{n}(0) + \bar{n}(0) + o(\lambda) = \tilde{n}(0)e^{-\tilde{\psi}(0)} + o(\lambda) \quad (4.30) (a)$$

$$p(0, \lambda) = \tilde{p}(0) + \hat{p}(0) + o(\lambda) = \tilde{p}(0)e^{\tilde{\psi}(0)} + o(\lambda) \quad (4.30) (b)$$

holds. $\tilde{p}(0) = 0$ is impossible because of (4.24) (b).

Since $\psi_+ = \psi_+^0(\lambda) - \frac{U}{2U_T}$ holds, the reduced problem (4.23), (4.24) can be regarded as dependent on λ for $U \leq U_0$. We now prove an existence result for this case.

Theorem 4.3. Assume that $D \in C^1([0, 1])$ and $D(x) \geq M > 0$ on $[0, 1]$ and that

$$U \leq U_0, \quad U_0 < 2\psi_+^0(\lambda)U_T \quad (4.31)$$

holds. Moreover if

$$\lambda \leq \lambda_0 = \lambda_0\left(\frac{U_0}{U_T}\right) \quad (4.24)$$

holds, then the reduced problem (4.23), (4.24) has a locally unique solution fulfilling

$$\begin{aligned}
(a) \quad \tilde{\psi}(x) &= \psi_+ + \ln D(x) + O\left(\frac{1}{\psi_+^2}\right) & \psi_+ \rightarrow \infty \\
(b) \quad \tilde{n}(x) &= D(x) + O\left(\frac{1}{\psi_+^2}\right) & \psi_+ \rightarrow \infty \\
(c) \quad \tilde{p}(x) &= O\left(\frac{1}{\psi_+^2}\right) & \psi_+ \rightarrow \infty \\
(d) \quad \tilde{J}_n(x) &= O\left(\frac{1}{\psi_+^2}\right) & \psi_+ \rightarrow \infty \\
(e) \quad \tilde{J}_p(x) &= O\left(\frac{1}{\psi_+^2}\right) & \psi_+ \rightarrow \infty
\end{aligned} \tag{4.25}$$

Proof. We substitute $\tilde{\varphi} = \frac{1}{\tilde{\psi}} - \frac{1}{\psi_+}$, set $\varphi_+ = \frac{1}{\psi_+}$ and get from (4.23) (b), (4.24) (b), (c)

$$\tilde{\varphi}' = -(\tilde{\varphi} + \varphi_+)^2 \frac{D' - (\tilde{J}_n + \tilde{J}_p)}{2\tilde{n} - D} \tag{4.26} (a)$$

$$\tilde{n}(0) \exp\left(-\frac{2}{\tilde{\varphi}(0) + \varphi_+}\right) - (\tilde{n}(0) - D(0)) = 0 \tag{4.26} (b)$$

$$\tilde{\varphi}(1) = 0. \tag{4.26} (c)$$

We rewrite the reduced problem in operator form $F_{\varphi_+}(\tilde{z}) = 0$ where $F_{\varphi_+} : \Omega \subset (C^1([0, 1]))^4 \rightarrow (C([0, 1]))^4 \times \mathbb{R}^4$, Ω open and $\tilde{z} = (\tilde{\varphi}, \tilde{n}, \tilde{J}_n, \tilde{J}_p)$:

$$\begin{aligned}
F_{\varphi_+}(\tilde{z}) &= (\tilde{\varphi}' + (\tilde{\varphi} + \varphi_+)^2 \frac{D' - (\tilde{J}_n + \tilde{J}_p)}{2\tilde{n} - D}, \tilde{n}' - \frac{n(D' + \tilde{J}_n - \tilde{J}_p) - D\tilde{J}_n}{2\tilde{n} - D}, \tilde{J}_n' - \frac{1}{4} \frac{\tilde{n}(\tilde{n} - D)}{2\tilde{n} - D}, \\
&\quad \tilde{J}_p' + \frac{1}{4} \frac{\tilde{n}(\tilde{n} - D)}{2\tilde{n} - D}, \tilde{\varphi}(1), \tilde{n}(1) - 1, \tilde{J}_p(0) - \tilde{J}_n(0),
\end{aligned} \tag{4.27}$$

$$\tilde{n}(0) \exp\left(-\frac{2}{\tilde{\varphi}(0) + \varphi_+}\right) - (\tilde{n}(0) - D(0)) = 0.$$

The spaces are equipped with their natural norms (see Appendix A).

We define

$$\tilde{z}_0 = (0, D, 0, 0) \in \Omega \quad (4.28)$$

and evaluate F_{φ_+} at \tilde{z}_0 :

$$F_{\varphi_+}(\tilde{z}_0) = \left(\frac{\varphi_+^2 D'}{D}, 0, 0, 0, 0, 0, 0, D(0) \exp\left(-\frac{2}{\varphi_+}\right) \right). \quad (4.29)$$

This yields consistency

$$\|F_{\varphi_+}(\tilde{z}_0)\| \leq \text{const. } \varphi_+^2 \text{ as } \varphi_+ \rightarrow 0+. \quad (4.30)$$

We calculate the linearization $F'_{\varphi_+}(\tilde{z}_0)$ and investigate the equation

$F'_{\varphi_+}(\tilde{z}_0) = (f, \omega)$, $f \in (C([0, 1]))^4$, $\omega \in \mathbb{R}^4$. So we obtain the linear boundary-value problem:

$$y' = \begin{bmatrix} -2\varphi_+ \frac{D'}{D} & 2\varphi_+^2 \frac{D'}{D^2} & \frac{\varphi_+^2}{D} & \frac{\varphi_+^2}{D} \\ 0 & -\frac{D'}{D} & 0 & -1 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \end{bmatrix} y + f, \quad 0 \leq x \leq 1 \quad (4.31)(a)$$

$$y_1(1) = \omega_1$$

$$y_2(1) = \omega_2$$

(4.31) (b)

$$y_3(0) - y_4(0) = \omega_3$$

$$\frac{2}{\varphi_+} \frac{D(0)}{2} \exp\left(-\frac{2}{\varphi_+}\right) y_1(0) + \left(\exp\left(-\frac{2}{\varphi_+}\right) - 1\right) y_2(0) = \omega_4.$$

The perturbed problem

$$u' = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -\frac{D'}{D} & 0 & -1 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \end{bmatrix} u + g, \quad 0 \leq x \leq 1 \quad (4.32) (a)$$

$$u_1(1) = \rho_1$$

$$u_2(1) = \rho_2$$

(4.32) (b)

$$u_3(0) - u_4(0) = \rho_3$$

$$u_2(0) = \rho_4$$

has a unique solution for all $g \in (C([0,1]))^4$, $\rho \in \mathbb{R}^4$ fulfilling

$$\|u\|_{[0,1]} + \|u'\|_{[0,1]} \leq \text{const.} (\|f\|_{[0,1]} + \sum_{i=1}^4 |\rho_i|) \quad (4.33)$$

iff the homogeneous problem

$$v_1' = -(\ln D)' v_1 - v_3$$

$$v_2' = \frac{1}{4} v_1 \quad (4.34) (a)$$

$$v_3' = -\frac{1}{4} v_1$$

$$v_1(1) = 0, \quad v_1(0) = 0, \quad v_2(0) = v_3(0) \quad (4.34) (b)$$

has only the trivial solution $v \equiv 0$. This holds iff

$$y'' + (\ln D)' y' - \frac{1}{4} y = 0, \quad y'(0) = y'(1) = 0 \quad (4.34) (c)$$

has only the trivial solution $y \equiv v_3 \equiv 0$, which follows from the maximum principle since $M_1 \leq (\ln D)' \leq M_2$ holds.

The contraction mapping theorem assures the unique solvability of (4.31) (for φ_+ sufficiently small) for all $f \in (C([0,1]))^4$, $\omega \in \mathbb{R}^4$ and the stability estimate

$$\|y\|_{[0,1]} + \|y'\|_{[0,1]} \leq K_1 (\|f\|_{[0,1]} + \sum_{i=1}^4 |\omega_i|) \quad (4.35)$$

where K_1 is independent of φ_+ .

An easy calculation shows the uniform Lipschitz continuity of F'_{φ_+} locally around \tilde{z} .

$$\|F'_{\varphi_+}(\tilde{u}) - F'_{\varphi_+}(\tilde{v})\| \leq K_2 \|\tilde{u} - \tilde{v}\| \quad (4.36)$$

with $\|u - \tilde{z}_0\|, \|v - \tilde{z}_0\| \leq \rho$ and K_2 is independent of φ_+ . Applying Keller's (1975) theory we conclude that the equation $F'_{\varphi_+}(\tilde{z}) = 0$ has a locally unique solution $\tilde{z} = \tilde{z}(\varphi_+)$ if $\varphi_+ < c(K_1, K_2)$ which fulfills

$$\|\tilde{z}(\varphi_+) - \tilde{z}_0\|_{[0,1]} + \|\tilde{z}'(\varphi_+) - \tilde{z}'_0\|_{[0,1]} \leq \text{const. } \varphi_+^2. \quad (4.37)$$

This translates immediately into the existence statement given in Theorem 4.3 (using $\varphi_+ = \frac{1}{\psi_+(\lambda) - \frac{U}{2U_T}}$). (4.25(b)-(e) follow from (4.37) and (4.25)(a) follows from (4.23)(a).

If $D \equiv 1$ then the first component in $F_{\varphi_+}(\tilde{z}_0)$ is zero and instead of (4.30) we get

$$\|F_{\varphi_+}(\tilde{z}_0)\| = \exp(-\frac{2}{\varphi_+}). \quad (4.38)$$

Therefore the $O(\frac{1}{\psi_+})$ -terms in (4.25) can be substituted by $O(\exp(-2\psi_+))$ and the bound λ_0 in (4.24) can be chosen larger.

Questions that arise are whether the asymptotic expansion (4.10) actually represents a solution of (2.6), (2.10) and whether (4.10) is uniform in ψ_+ in some sense (this is particularly interesting in context with Theorem 4.3). For simplified pn-junction models the first question was positively answered by D. Smith (1980), Vasileva and Butuzow (1978) and Vasileva and Stelmakh (1977). For a validity proof of the asymptotic expansion (4.10) (for $\psi_+ = O(1)$ as $\lambda \rightarrow 0+$) one has to proceed similarly to the references cited above (particularly Vasileva and Butuzow (1978)).

Our numerical experiments show that the expansions are valid in the sense that a numerical solution of (2.6), and (2.10) can be obtained by using the sum of the reduced solution and the boundary layer solution as initial guess for the numerical scheme for (2.6) and (2.10) and this obtained solution is close to the initial guess.

For the following computations the parameter values from Section 1 and $D(x) \equiv 1$ were taken.

Figures 5 through 7 show the reduced solutions $U_T \tilde{\psi}, \tilde{n}, \tilde{J}_n, \tilde{J}_p$ for $\psi_+ = 0$ which correspond to a forward bias $U = 0.806V$. The corresponding full solutions $U_T \psi, n, p$ (of (2.6), (2.10)) are shown in Figures 8 and 9. J_n and J_p are not shown since they differ inappreciably from \tilde{J}_n, \tilde{J}_p . Figures 10 and 11 show \tilde{J}_n, \tilde{J}_p for $U = 1.506V$ ($\psi_+ = -14$) and for $U = 0.306V$ ($\psi_+ = 10$) respectively. We get the following Table 2 for the total current $J = J_n + J_p \approx \tilde{J}_n + \tilde{J}_p$

ψ_+	U	J
10	0.306V	4.4×10^{-9}
0	0.806V	0.92
-14	1.506V	108.2

Table 2: Current-Voltage Relation

The characteristic curve $J = J(\frac{U}{U_T})$ behaves exponentially (see A. Smith (1978), Section 7.9).

The computations demonstrate that $\tilde{\psi}(0) \rightarrow 0$ as $\psi_+ \rightarrow -\infty$ and therefore the jump of the boundary layer of ψ tends to zero. Since

$$\bar{n}(0) = -D(0) \frac{e^{\tilde{\psi}(0)}}{e^{\tilde{\psi}(0)} + 1} \quad (4.39)(a)$$

$$\bar{p}(0) = D(0) \frac{1}{e^{\tilde{\psi}(0)} + 1} \quad (4.39)(b)$$

hold, the layer jumps of n and p tend to $\frac{D(0)}{2}$. This is illustrated by the Figures 12 and 13 which show the solutions $U_T \psi$ and n, p (of (2.6), (2.10)) respectively, for $\psi_+ = -14$ ($U = 1.506V$). No layer in $U_T \psi$ is visible and the layers

FIGURE 5 $U = 0.806V$ ($\psi_+ = 0$)

REDUCED SOLUTION PSI

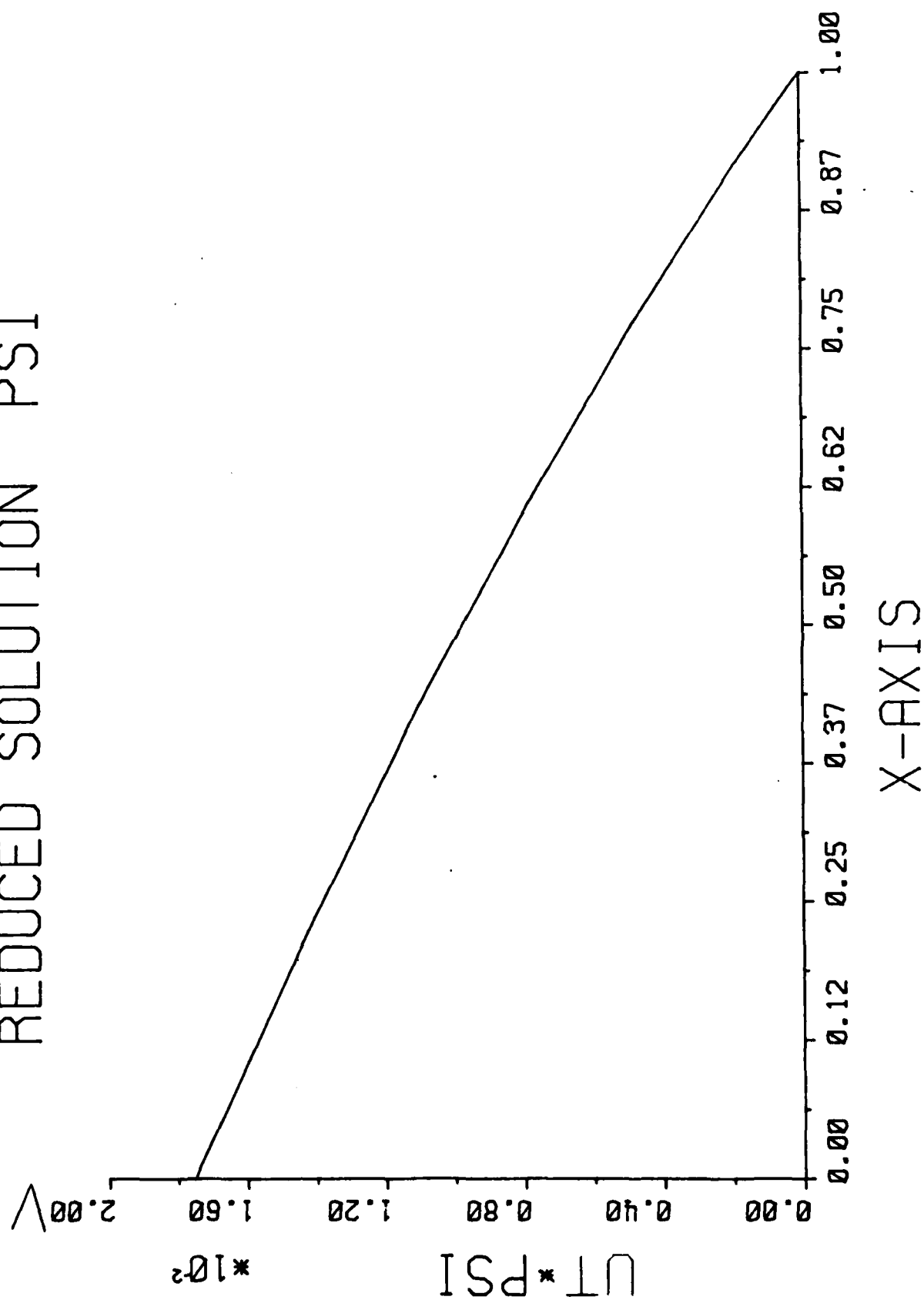


FIGURE 6 $V = 0.806V$ ($\psi_+ = 0$)

REDUCED SOLUTION N

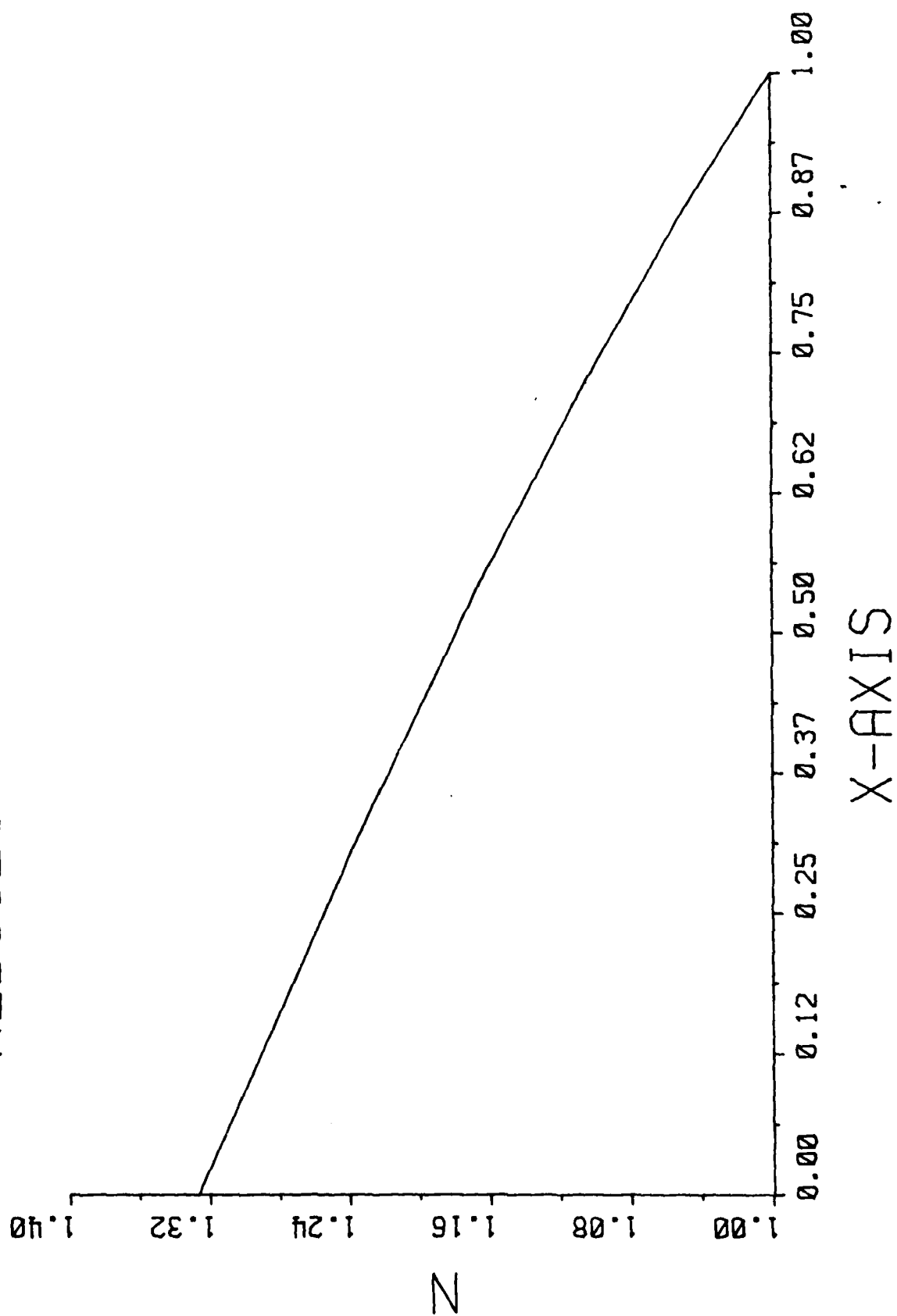


FIGURE 7 $U = 0.806V$ ($\psi_+ = 0$)

REDUCED SOLUTION JN, JP

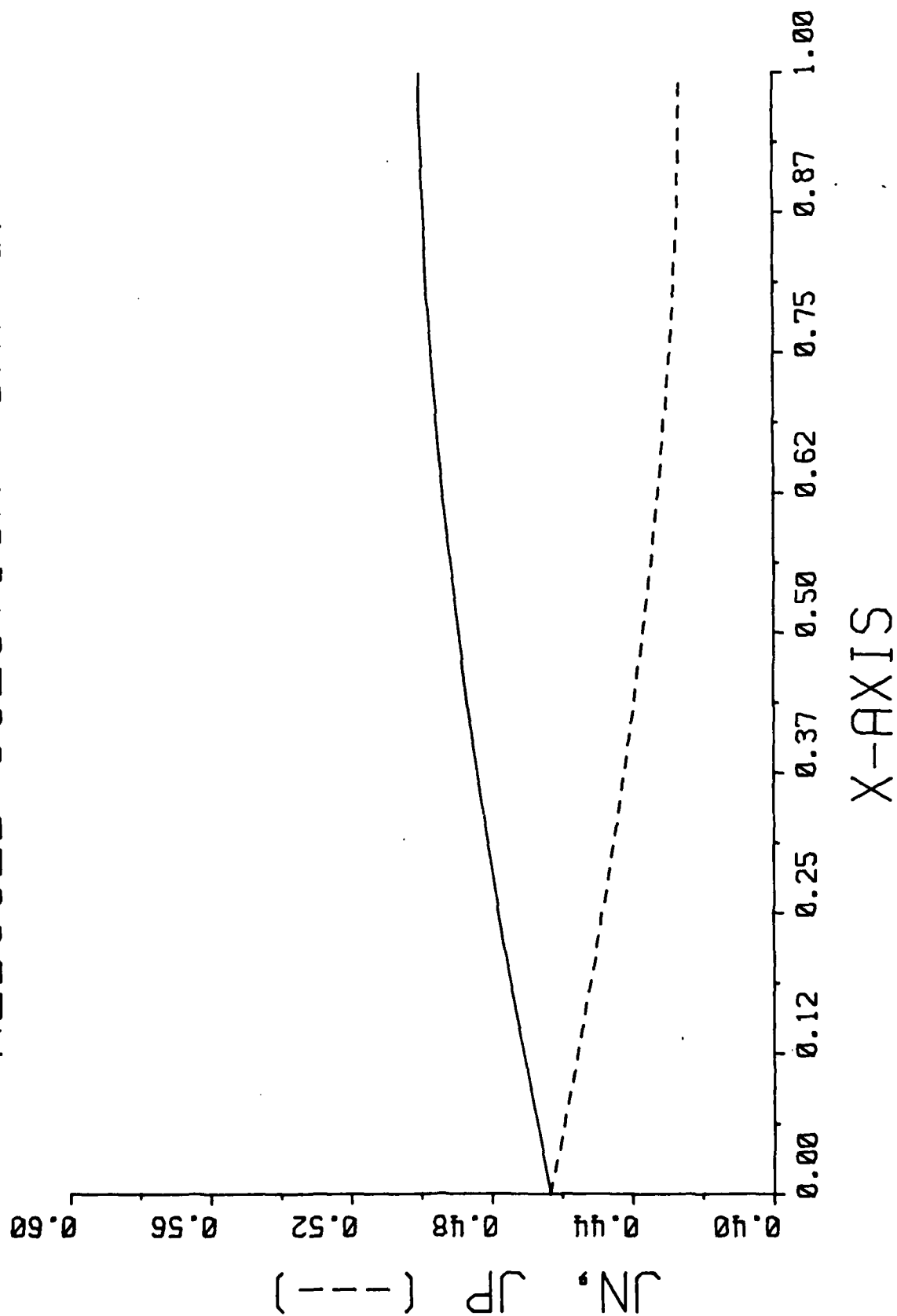


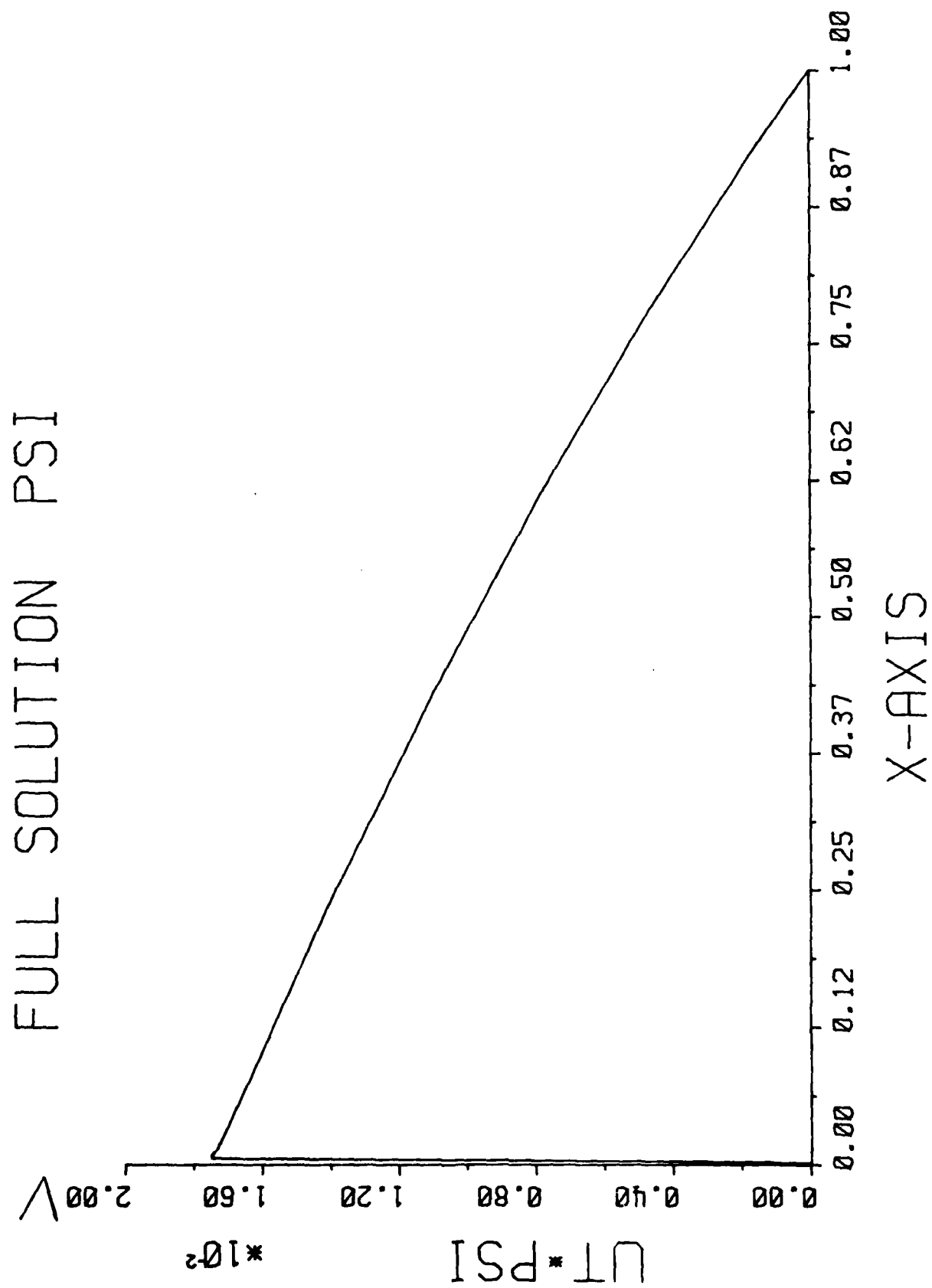
FIGURE 8 $U = 0.806V$ ($V_+ = 0$)

FIGURE 9 $U = 0.806V$ ($\psi_+ = 0$)

FULL SOLUTION N, P

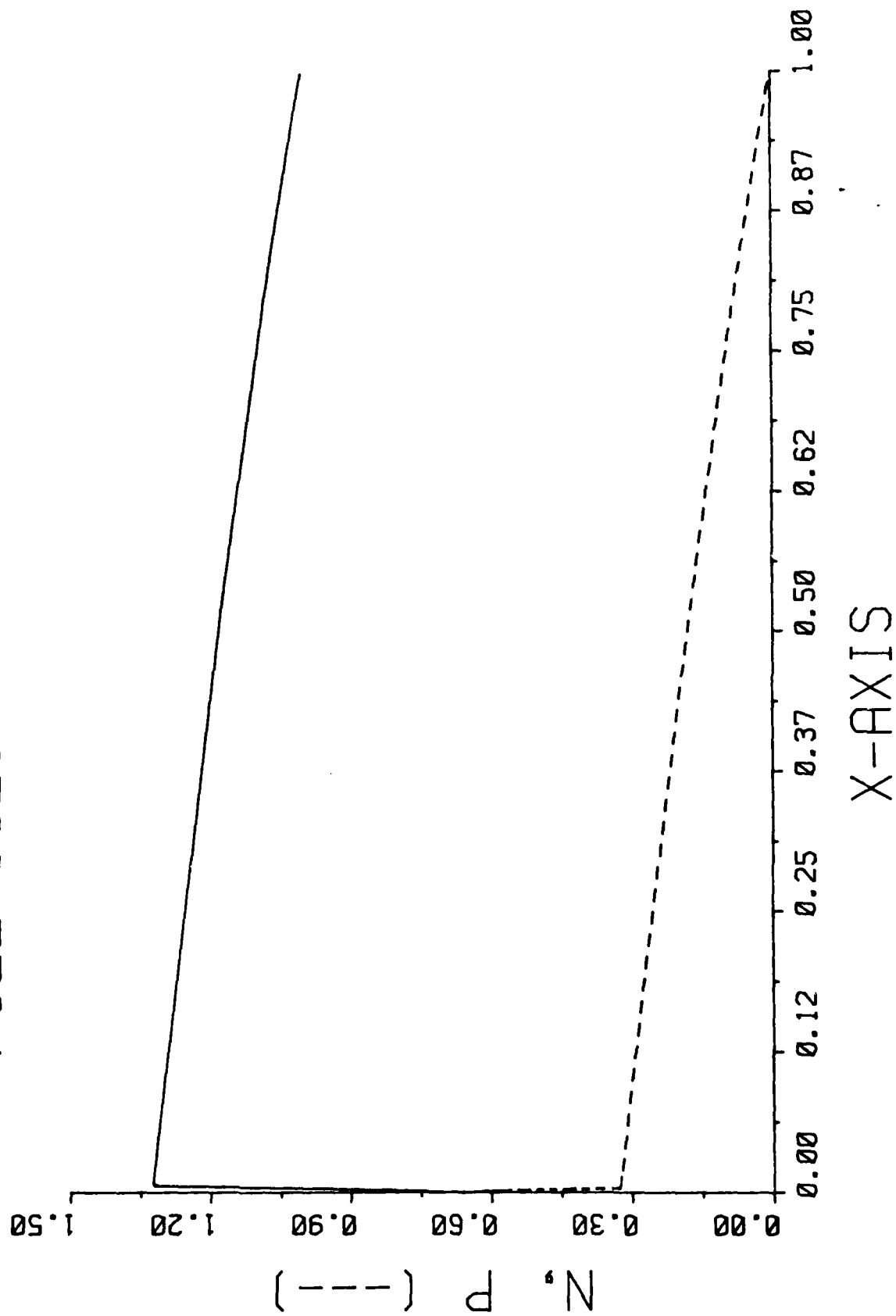


FIGURE 10 $U = 1.506V$ ($\psi_+ \approx -14$)

REDUCED SOLUTION JN, JP

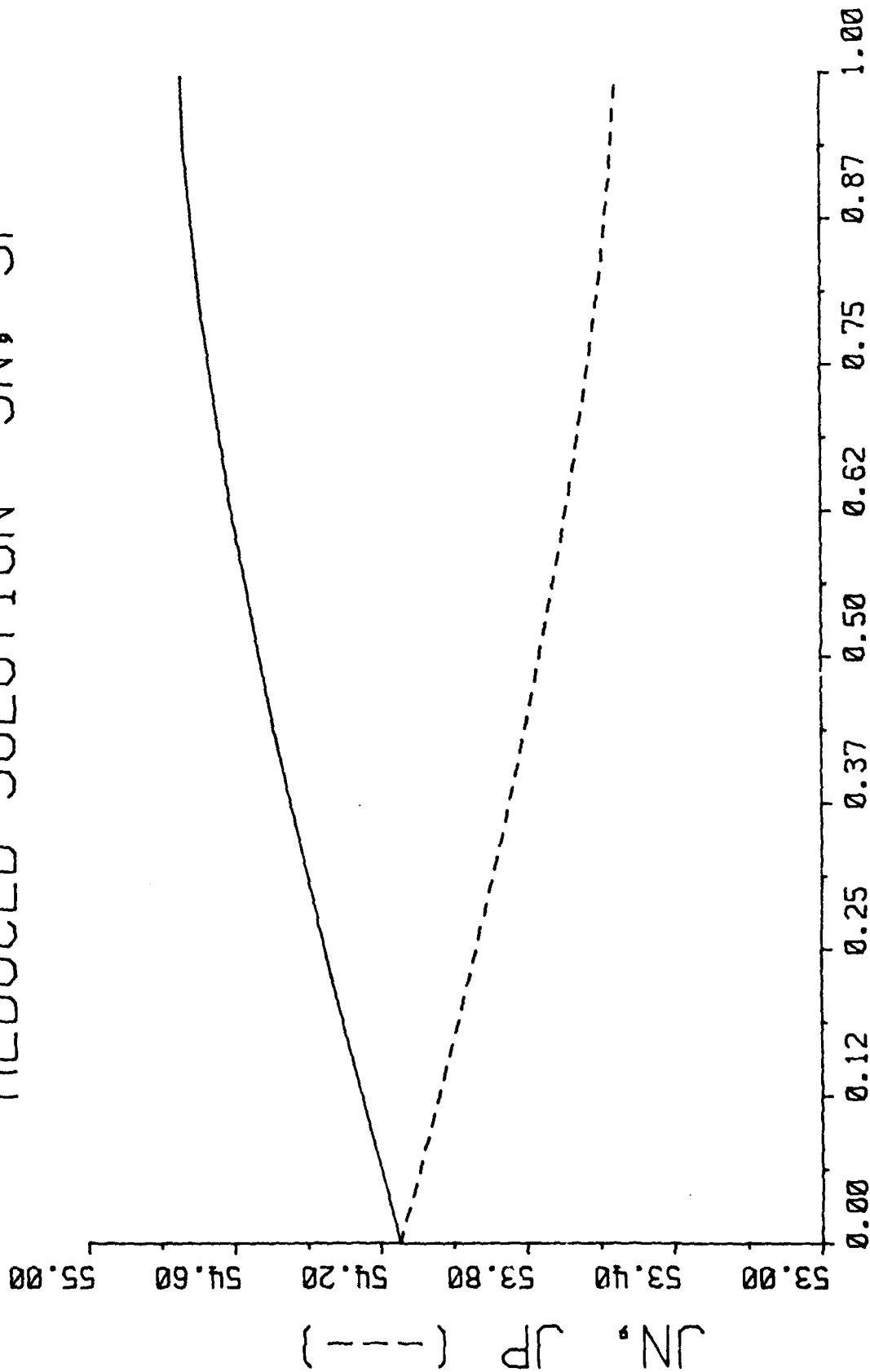


FIGURE 11 $U = 0.306V$ ($\Psi_+ = 10$)

REDUCED SOLUTION JN, JP

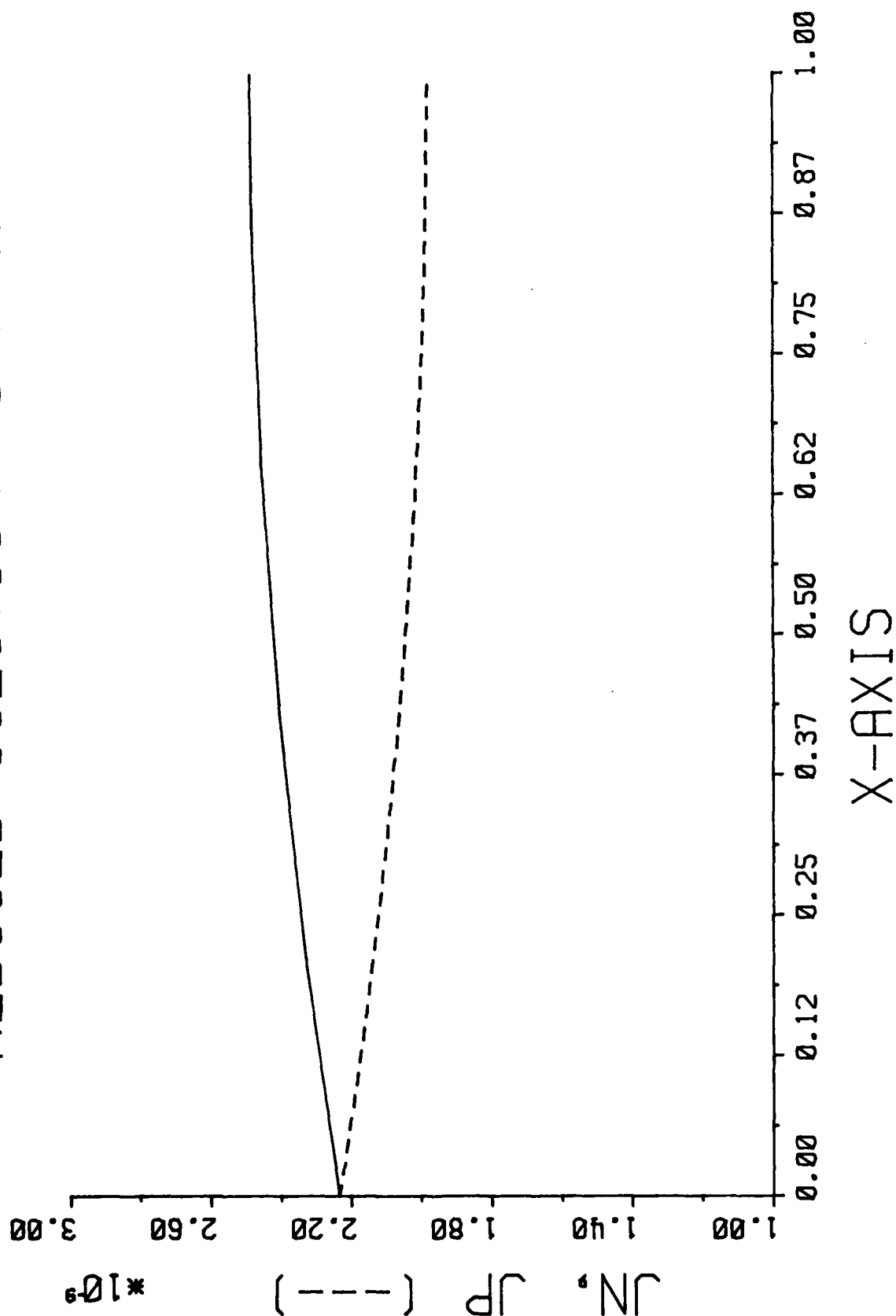


FIGURE 12 $U = 1.506V$ ($\psi_+ = -14$)

FULL SOLUTION PSI

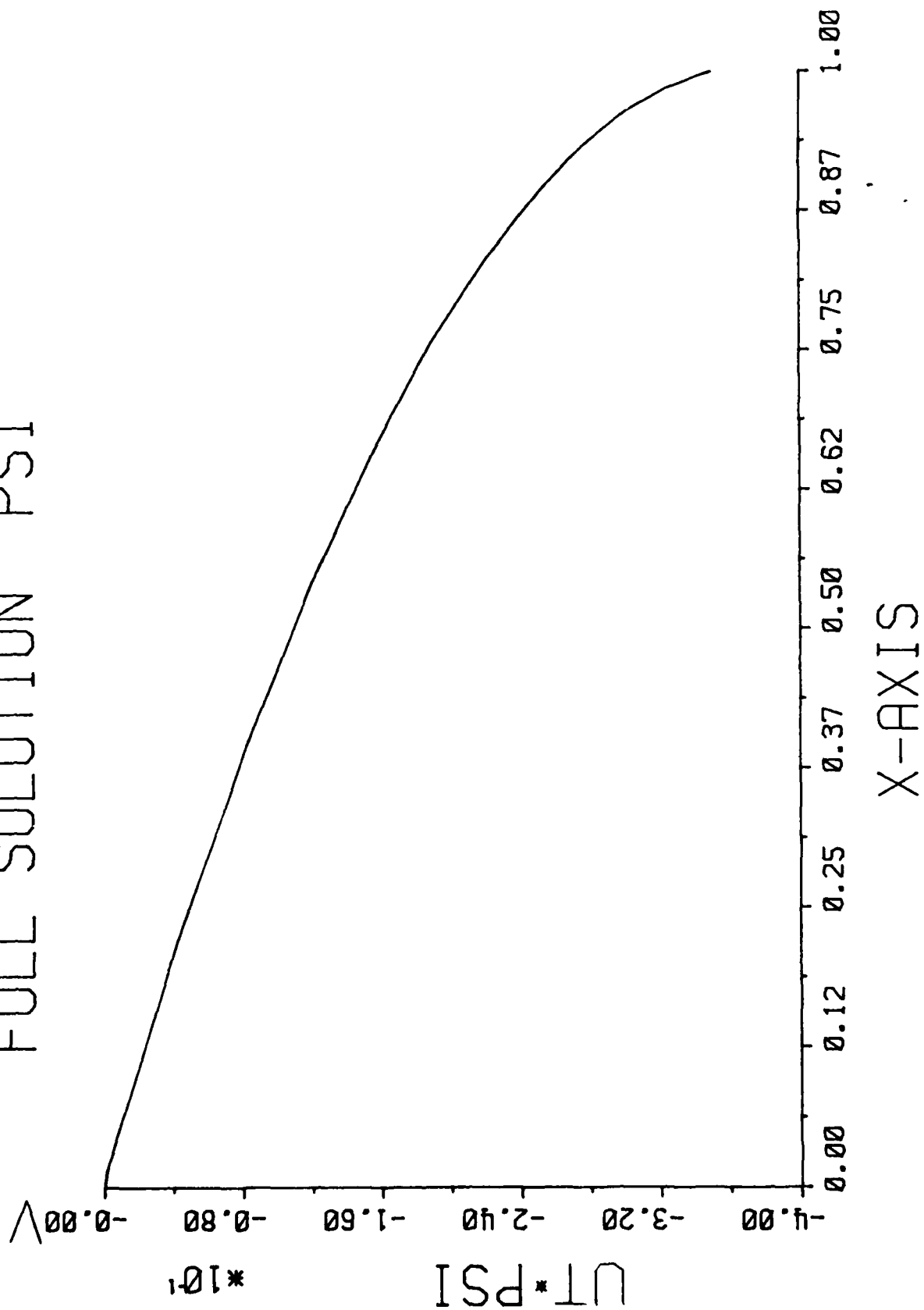
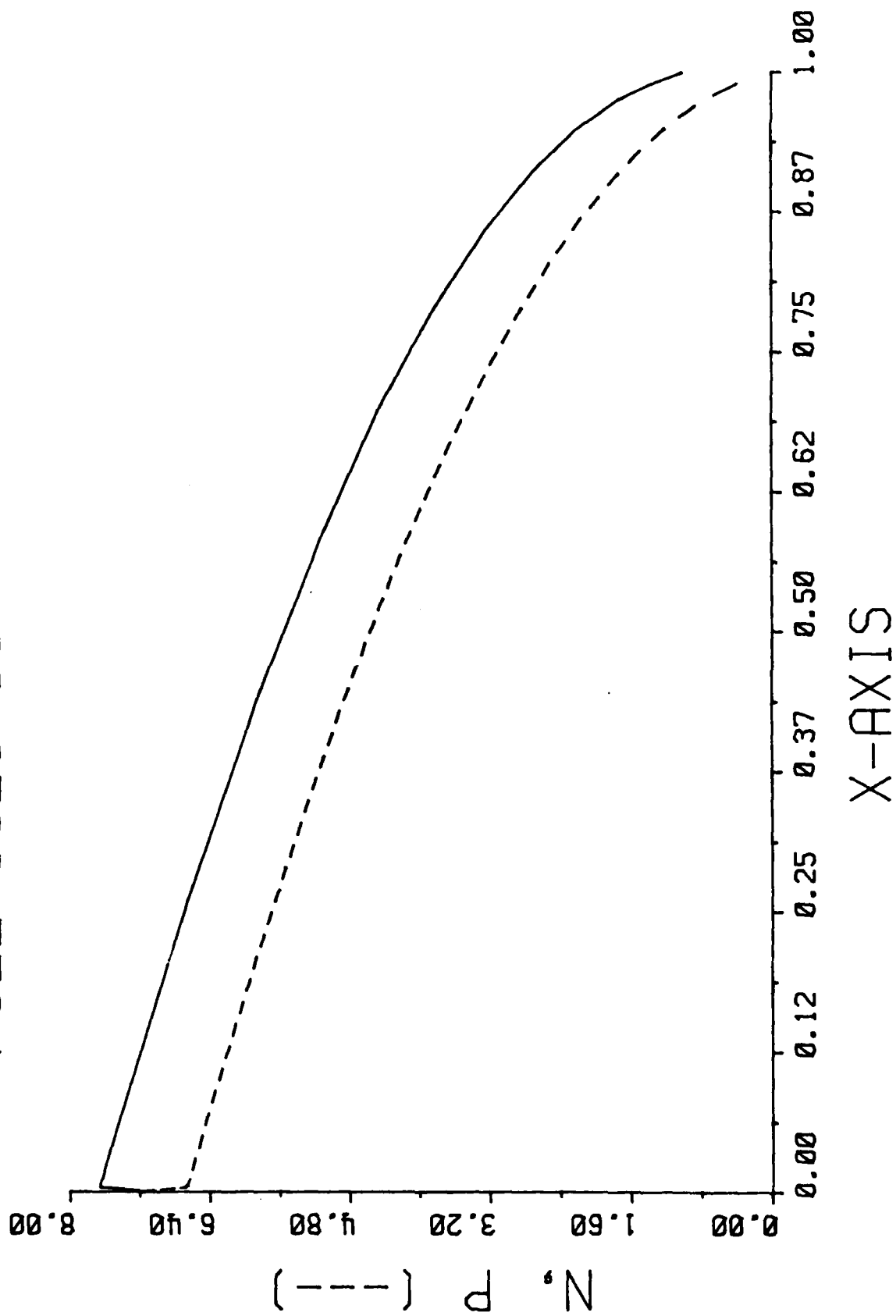


FIGURE 13 $U = 1.506V$ ($\psi_+ = -14$)FULL SOLUTION N, P 

of n, p are of approximate height 0.5 (see also Figure 14 which shows the corresponding boundary layer solutions \bar{n}, \bar{p}).

Figures 15 and 16 show the solutions $U_T \psi$ and n respectively with $U = 0.306V$ ($\psi_+ = 10$). The corresponding hole density p is nearly constant zero (indistinguishable from the x -axis). ψ and n are (disregarding the layers) nearly constant. The explanation for this behaviour is given by Theorem 4.3. Since $D(x) \equiv 1$ the estimate (4.25) can be strengthened (see remark to Theorem 4.3):

$$\|\tilde{\psi} - \psi_+\|_{[0,1]} + \|\tilde{n} - 1\|_{[0,1]} + \|\tilde{p}\|_{[0,1]} + \|\tilde{j}_n\|_{[0,1]} + \|\tilde{j}_p\|_{[0,1]} \leq \text{const.} (\exp(-2\psi_+)) \quad (4.40)$$

and $2\psi_+ = 20$.

Since $\tilde{\psi}(0) \sim \psi_+$ as $\psi_+ \rightarrow \infty$ the boundary layer jump of ψ grows at ψ_+ , the jump of the layer of n tends to $D(0)$ and the jump of the layer of p tends to zero exponentially (see (4.39)). The width of the depletion layer which is given by (4.29) grows logarithmically with ψ_+ for constant λ . Figures 17, 18, 19, 20 show the growth of the layer of $U_T \psi$. Figure 21 shows the boundary layer solution \hat{n} for $U = -19.194V$ (reverse bias). The depletion region is almost free of carriers (since $n \sim 1 + \hat{n}$, $p \sim 0$).

FIGURE 14 $U = 1.506$ ($\psi_+ = -14$)

LAYER SOLUTION N, P

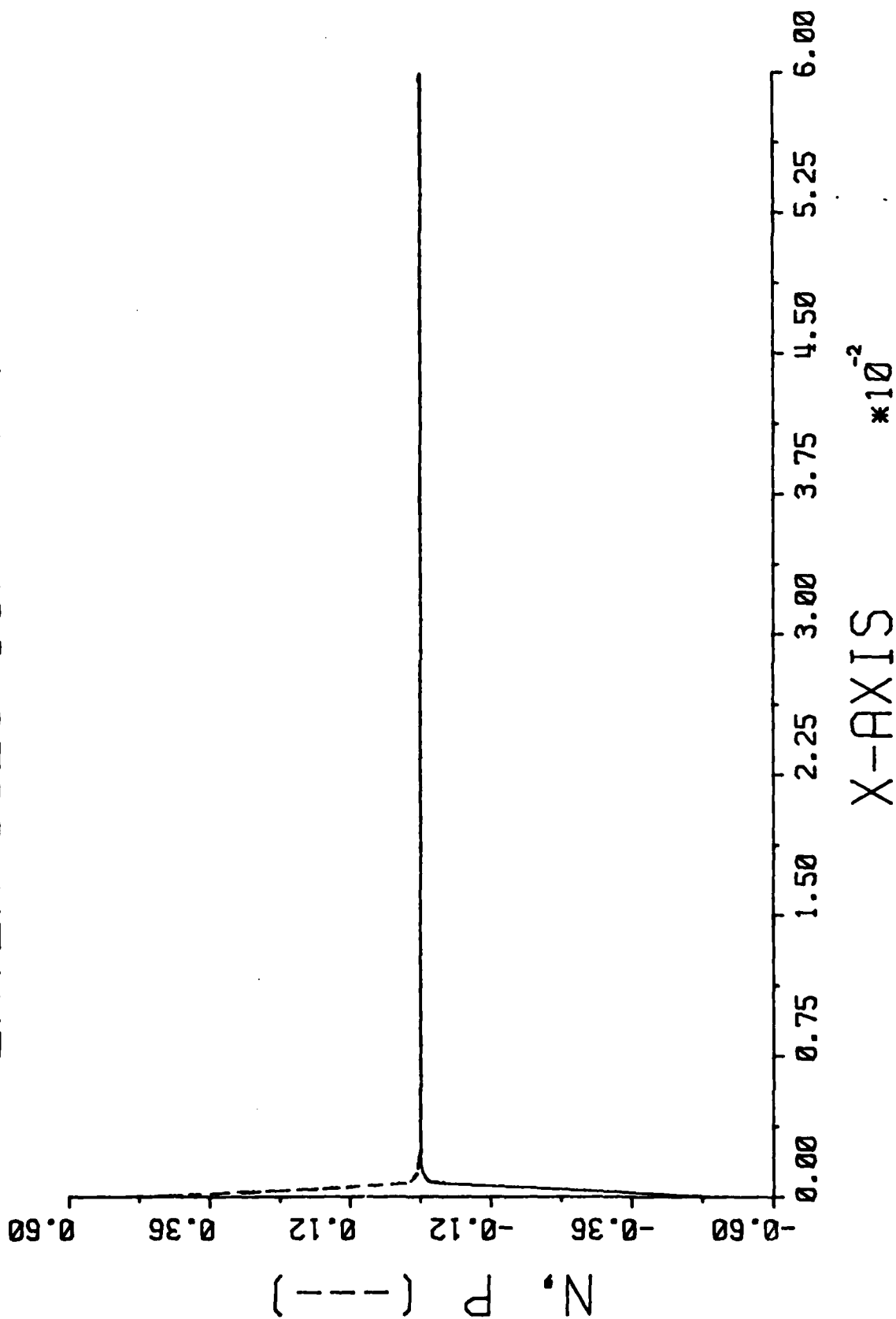


FIGURE 15 $U = 0.306V$ ($\psi_+ = 10$)

FULL SOLUTION PSI

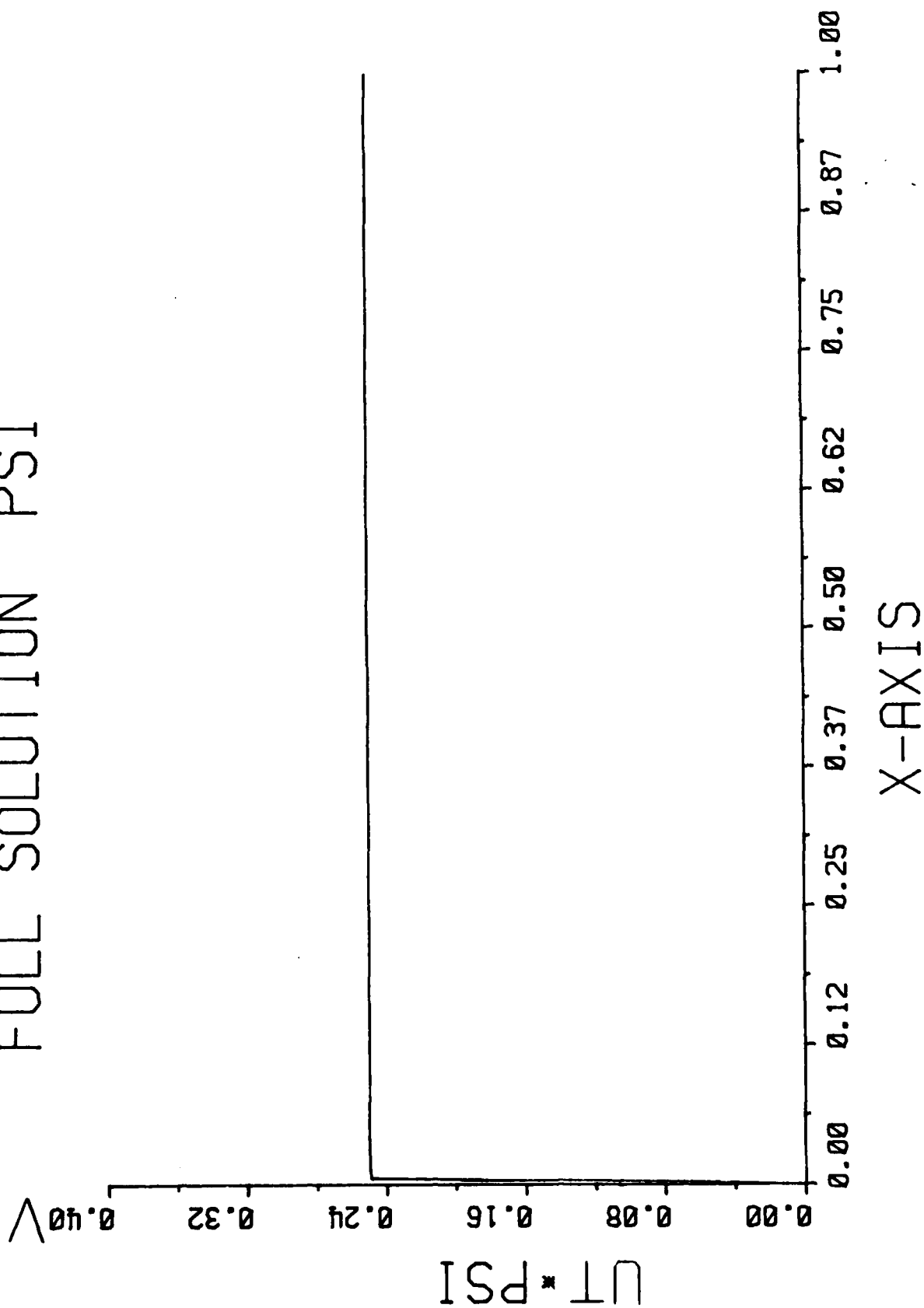


FIGURE 16 $U = 0.306V$ ($\psi_+ = 10$)

FULL SOLUTION N

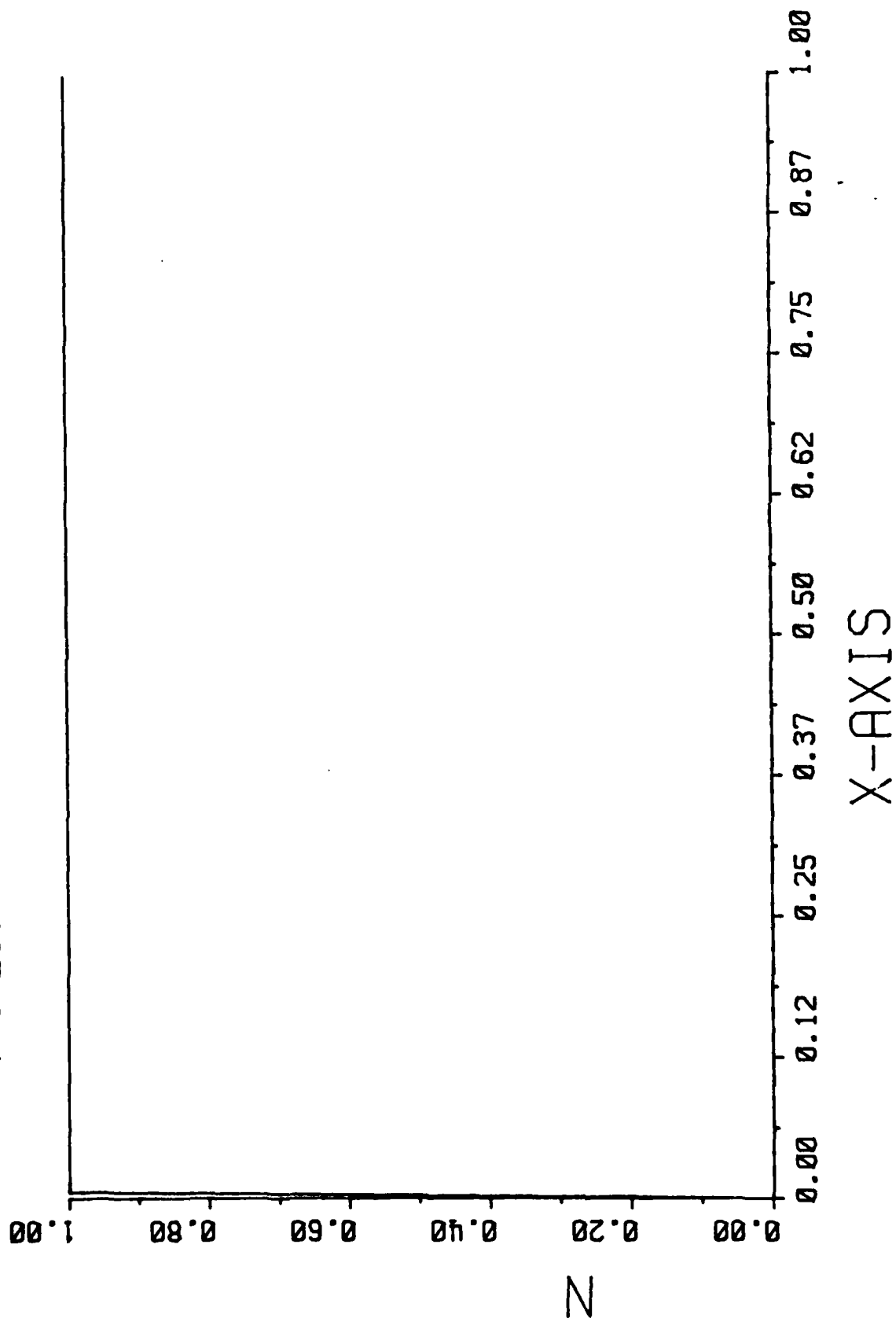


FIGURE 17 $U = 1.506V$ ($\psi_+ = -14$)

LAYER SOLUTION PSI

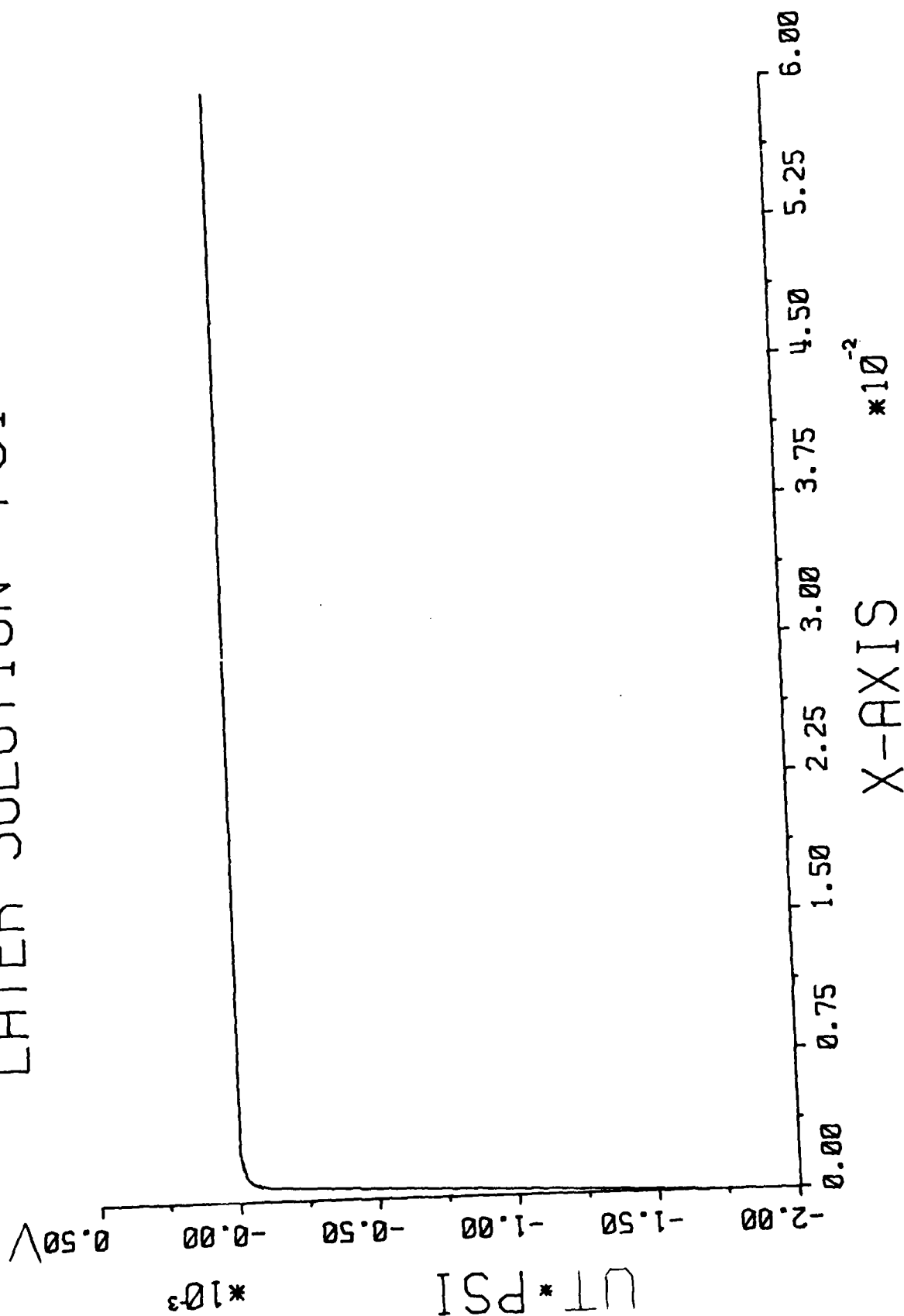


FIGURE 18 $U = 0.306V$ ($\psi_+ = 10$)

LAYER SOLUTION PSI

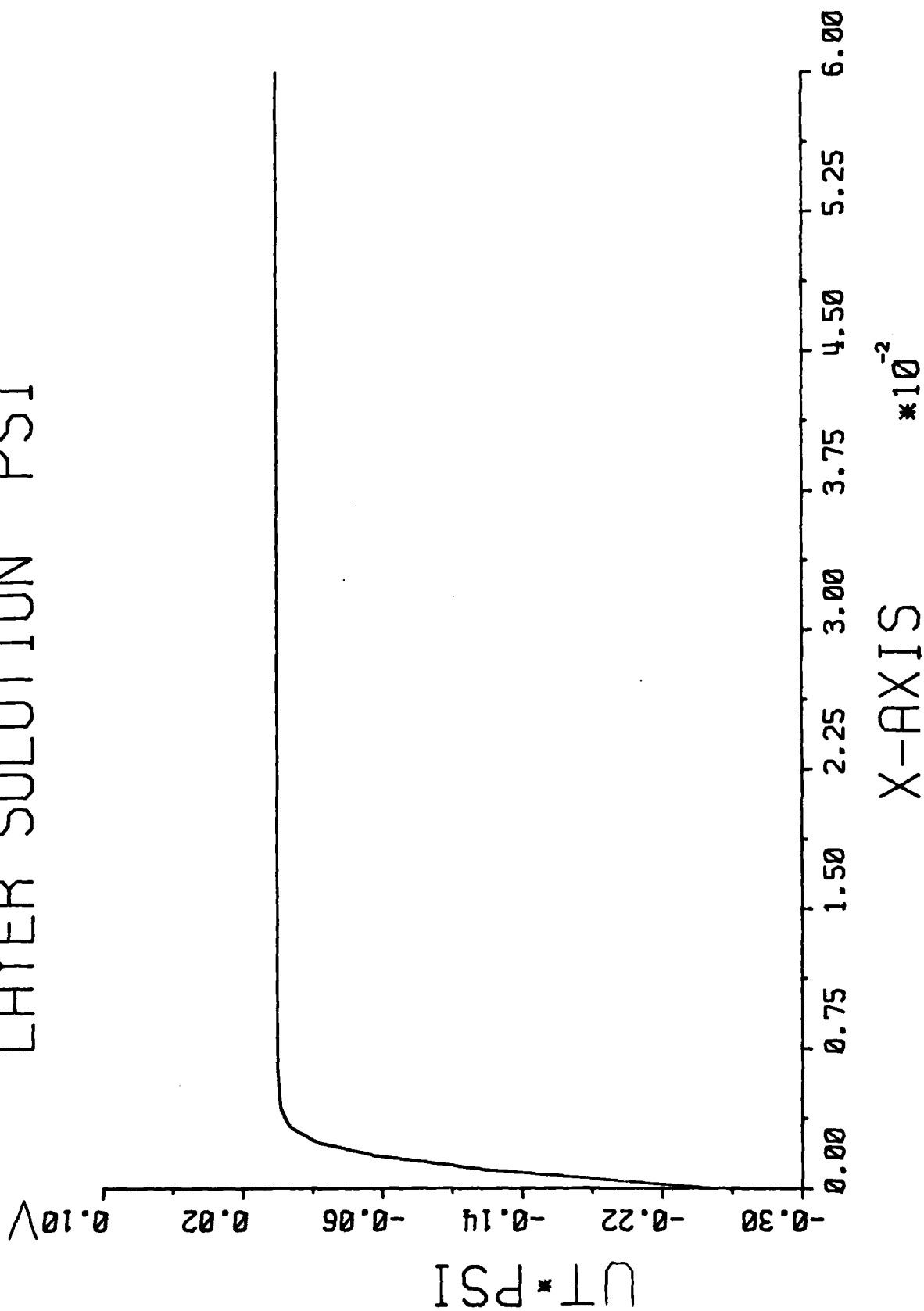


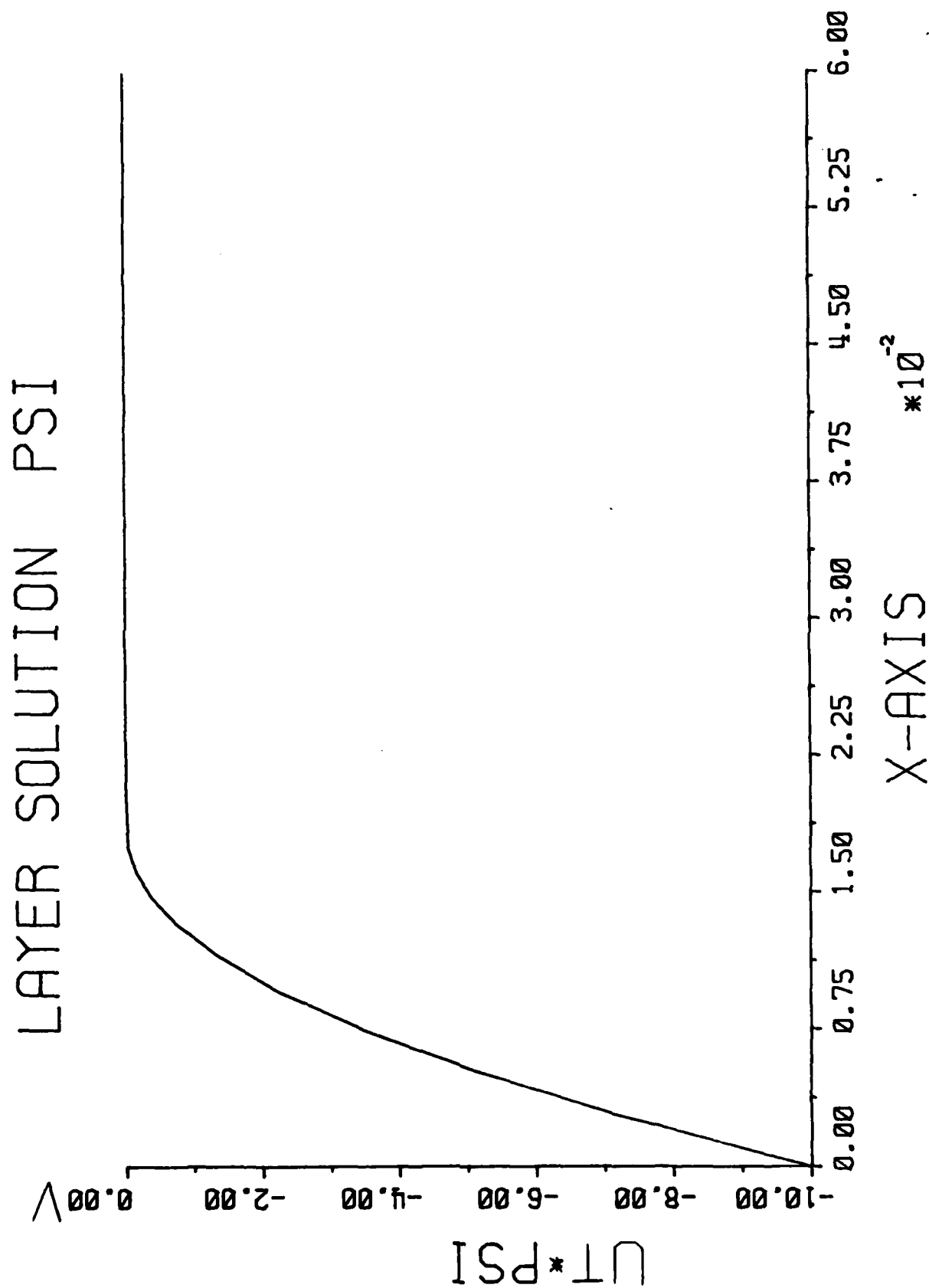
FIGURE 19 $U = -19.194V$ ($\psi_+ = 400$)

FIGURE 20 U = -99.194V ($\psi_+ = 2000$)

LAYER SOLUTION PSI

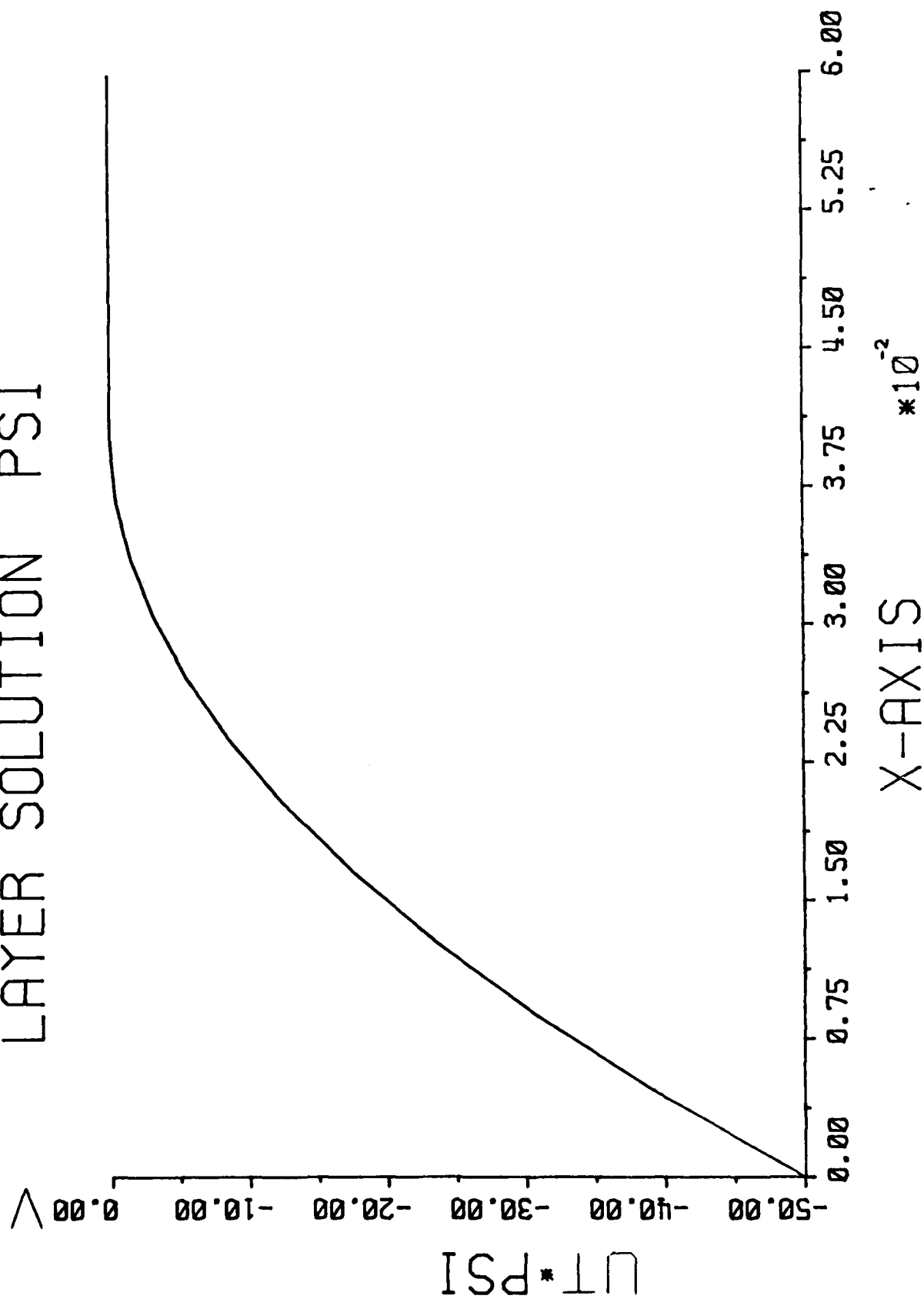
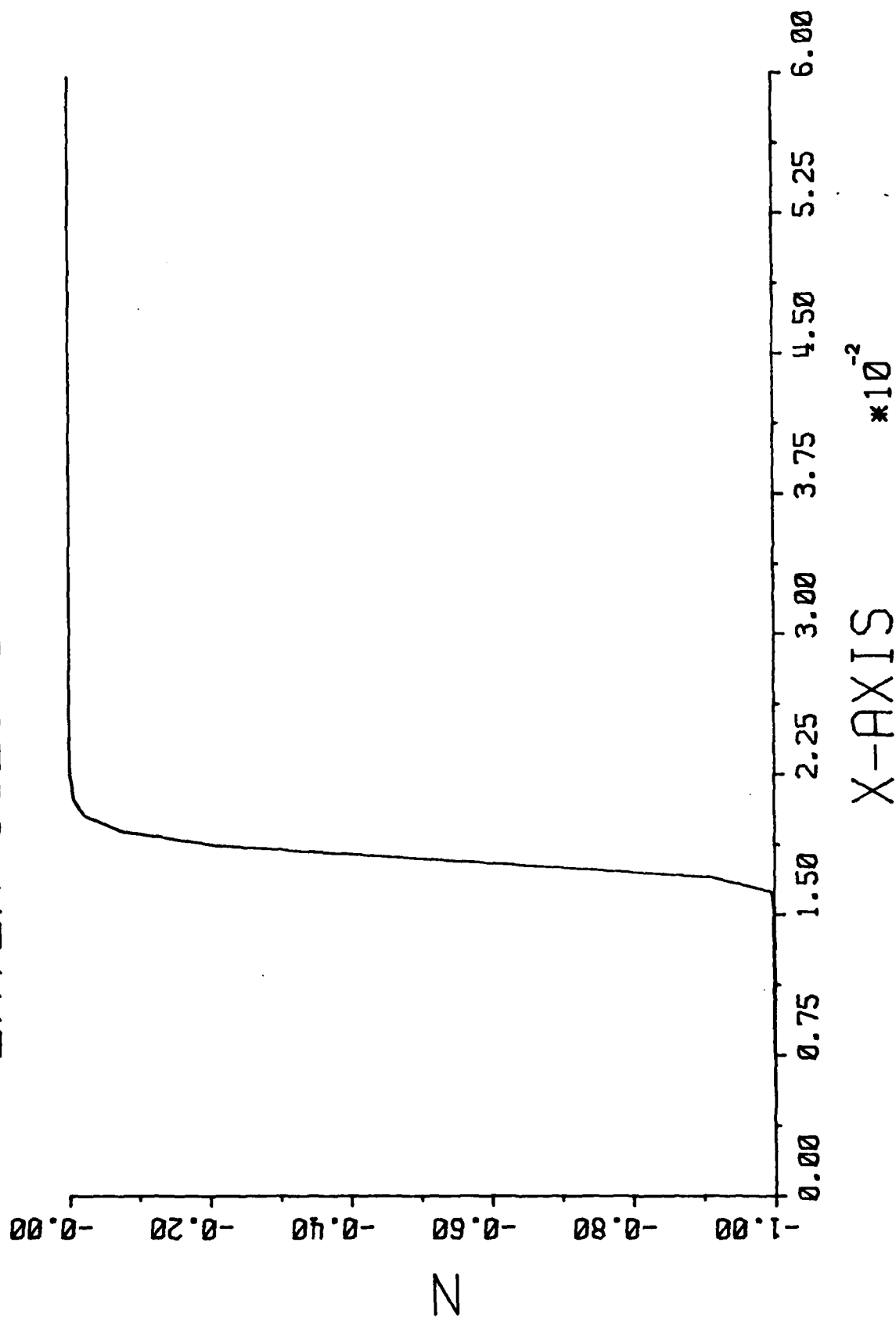


FIGURE 21 $U = -19.194V$ ($\psi_+ = 400$)

LAYER SOLUTION N



Appendix A

Proof of Theorem 3.2. We substitute

$$\psi = \psi_+(1-v) \quad (A1)$$

and the problem (3.7), (3.8) transforms to

$$F(\psi_+, \lambda, v)(x) = (\lambda^2 v'' - \frac{1}{\psi_+} (e^{\frac{-\psi_+(2-v)}{1-e} - \frac{-\psi_+ v}{-2\psi_+}} + 1), \quad v(0) = 1, \quad v(1) = 0). \quad (A2)$$

We denote

$$g(\psi_+, v) = \frac{1}{\psi_+} (e^{\frac{-\psi_+(2-v)}{1-e} - \frac{-\psi_+ v}{-2\psi_+}} + 1) \quad (A3)$$

with $g(\psi_+, 0) = 0$, $g_v(\psi_+, 0) = \frac{e^{\frac{-2\psi_+}{1-e} + 1}}{-2\psi_+} > 0$ for $\psi_+ > 0$. The boundary layer

equation for (A2), (A3) is given by

$$V'' = g(\psi_+, V), \quad 0 \leq y < \infty \quad (A4)$$

$$V(0) = 1, \quad V(\infty) = 0. \quad (A5)$$

By proceeding as in Fife (1973) (proof of lemma 2.1) we find that (A4), (A5) has a unique monotone solution $V = V_{\psi_+}$ fulfilling (for $\psi_+ \geq C_+ > 0$)

$$0 < V_{\psi_+}(y) \leq \exp((-1+\delta)y), \quad y \geq \text{const.} \ln \psi_+ \quad (A6)$$

where $0 < \delta < 1$ and the constant depends on δ only. The linearization of $F(\psi_+, \lambda, \cdot)$ (viewed as operator from $C^2([0,1])$ into $C([0,1]) \times \mathbb{R}^2$) at

$\hat{v}_{\psi_+}(x, \lambda) = v_{\psi_+}(\frac{x}{\lambda})$ is given by

$$(L(\hat{v}_{\psi_+}, \lambda)y)(x) = (\lambda^2 y''(x) - g_{\psi_+}(\hat{v}_{\psi_+}(x, \lambda))y(x), y(0), y(1)) . \quad (A7)$$

In $C^1([0, 1])$ we take $\|u\| = \sum_{j=0}^1 \lambda^j \|u^{(j)}\|_{[0, 1]}$ for the following. Analogously to Fife (1973), Lemma 2.5, we get

$$\|L^{-1}(\hat{v}_{\psi_+}, \lambda)\| \leq \text{const. } \lambda^{-1} e^{\psi_+} \quad (A8)$$

where the constant is independent of λ, ψ_+ . Moreover, the linearization L fulfills

$$\|L(U, \lambda) - L(V, \lambda)\| \leq \text{const. } \psi_+ e^{\theta \psi_+} \|U - V\| \quad (A9)$$

for $\|U - \hat{v}_{\psi_+}\|, \|V - \hat{v}_{\psi_+}\| \leq \theta < 1$.

By inserting \hat{v}_{ψ_+} into (A2) we get using (A6)

$$\|F(\psi_+, \lambda, \hat{v}_{\psi_+})\| \leq \exp\left(\frac{(-1+\delta)}{\lambda}\right) . \quad (A10)$$

From Spijker (1972) we conclude that (A2) has a locally unique solution v if

$$\exp\left(\frac{(-1+\delta)}{\lambda}\right) \cdot (\psi_+ e^{\theta \psi_+} + \lambda^{-2} e^{2\psi_+}) < \rho \quad (A11)$$

for some ρ sufficiently small. Then

$$\|v - \hat{v}_{\psi_+}(x, \lambda)\| \leq \text{const. } \lambda^{-1} \exp\left(\psi_+ + \frac{(-1+\delta)}{\lambda}\right) \quad (A12)$$

holds. (A11) follows immediately from (3.9) and (3.10) follows from (A12) by using (A1).

Theorem 3.1 is a special case of Theorem 3.2 with $\psi_+ = \psi_+^0(\lambda)$. (3.9) holds, therefore (3.4), (3.5) follow immediately.

Proof of Theorem 3.3. Again we substitute

$$\psi = \psi_+(1-v) \quad (\text{A13})$$

and get from (3.15), (3.8)

$$\lambda^2 v'' = \frac{1}{\psi_+} (1 + p(1, \lambda) e^{\psi_+ v} - n(1, \lambda) e^{-\psi_+ v}) , \quad 0 \leq x \leq 1 \quad (\text{A14})$$

$$v(0) = 1 , \quad v(1) = 0 . \quad (\text{A15})$$

The reduced equation (A14) has the solution $\bar{v} \equiv 0$. From Fife (1973) we conclude that the semi-reduced problem

$$\lambda^2 w'' = \frac{1}{\psi_+} (1 - e^{-\psi_+ w}) , \quad 0 \leq x \leq 1 \quad (\text{A16})$$

$$w(0) = 1 , \quad w(1) = 0 \quad (\text{A17})$$

which is obtained by setting $\lambda = 0$ in the right hand side of (A14), has a solution fulfilling

$$w(x, \lambda) = O(\exp(\frac{1}{\lambda}(-1+\delta)x)) + O(\exp(-\frac{c}{\lambda})) , \quad c > 0 , \quad 0 < \delta < 1 \quad (\text{A18})$$

if λ is sufficiently small (depending on ψ_+). From Ringhofer (1980), (1981) we conclude that the linearization of (A16), (A17) at $w(x, \lambda)$ is uniformly stable with respect to λ . Since $p(1, \lambda) = O(\lambda^4)$ holds we get (3.16) by a simple perturbation argument (similar to the proof of Theorem 3.2).

Remark. Theorem 3.3 is not formulated uniformly in ψ_+ .

Appendix B

For the numerical solution of two-point boundary value problems we used polynomial collocation at Gaussian points (see de Boor and Swartz(1973), Russell (1974) and Weiss (1974)). This method translates into a system of (nonlinear) difference equations (if the two-point boundary value problem is nonlinear) which has to be solved numerically by an iterative method (for example Newton's method) starting from an initial guess for the solution (which has to be sufficiently accurate for the iteration to converge).

The order of convergence depends on the number k of collocation points in each subinterval. For Gauss points the global error at the grid points is an $O(h^{2k})$ where h is the maximal mesh size assuming that the linearized system of difference equations has a uniformly (as $h \rightarrow 0$) bounded inverse.

We used the code COLSYS (see Ascher, Christiansen and Russell (1973) and Ascher (1981)) as collocation solver with $k=3$ or $k=4$.

A problem affecting stability and consistency of the collocation scheme is the choice of the mesh. COLSYS is a completely adaptive code refining an initial mesh automatically in order to achieve a prescribed error tolerance. However, we did not use this option for solving boundary layer problems. Instead we prescribed a mesh which is exponentially graded in the layer region and coarse outside (where the solution is close to reduced solution) (see Ascher and Weiss (1981)). This mesh equidistributes the local discretization error and employs only a reasonable number of mesh points (error estimates and estimates on the number of mesh points are given in Markowich and Ringhofer (1981) for a similar class of problems).

The boundary layer equations (4.25), (4.26) were solved by cutting the infinite interval at a finite, far out point and by substituting an additional boundary condition at this point for the condition at infinity (see Markowich (1981) and Markowich and Ringhofer (1981)).

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ABSTRACT (cont.)

We analyse the equilibrium case (zero bias applied) and set up approximate models, posed as singularly perturbed second order equations, by neglecting the hole and electron current densities. This makes sense for small forward bias and for reverse bias.

For the full problems we prove an a priori estimate on the number of electron-hole carrier pairs and derive asymptotic expansions (as the perturbation parameter tends to zero) by setting up the reduced system and the boundary layer system. We prove existence theorems for both systems and use the asymptotic expansion to solve the model equations numerically and analyse the dependence of the solutions on the applied bias.

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